BONDED-PARTICLE MODELING OF THERMALLY INDUCED DAMAGE IN ROCK

By

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A thesis submitted in conformity with the requirements for obtaining the degree of Doctor of Philosophy

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Abstract: Bonded-particle modeling of thermally induced damage in rock, PhD, 2009, Toivo Wanne, Graduate Department of Civil Engineering, University of Toronto

The objective of the research presented in this thesis is to validate the parallel-bonded modeling method in the context of coupled thermo-mechanical simulations. The simulation results were compared with analytical and experimental data, in the attempt to assess the usability of this particular modeling method. Previous studies of numerical approaches that related to the thermal fracturing of hard rock had used continuum-based models with constitutive relations. The simulations in the thesis were conducted using Particle Flow Code (PFC) which was chosen for the research because of its several benefits. The code has unique features such as spontaneous damage development without imposed conditions, and emergent properties such as material heterogeneity, and dynamic behavior giving possibility to monitor synthetic seismic events. The basic code has been available since 1995 and research using the code has produced hundreds of publications. The thermal option for the code is a recent addition and lacked verification, validation and applications. The thesis is the answer for that. In the course of the research work new particle clustering and grouping routines were developed and tested. Three modeling studies were conducted varying from laboratory to field scales. The 2D modeling study of the heated cylinder experiment yielded similar results both in fracture-behavioral and acoustic emission (AE) magnitude ranges when compared with the laboratory data. The 3D cubic numerical specimens, created with breakable particle clusters, were heated, and the induced damage was observed by P wave velocity measurements. The results showed trends comparable to the laboratory data: P wave velocity decreases with rising temperatures of up to 250°C and cluster-boundary cracking occurs, comparable to grain-boundary cracking in the heated rock samples. The large 2D
tunnel models captured the phenomena observed in-situ displaying the difference in the damage to the roof and floor regions, respectively. This damage was due to the filling material confinement of about 100 kPa on the tunnel floor. In general, the results of the thermo-mechanical simulations were in accordance with the experimental data. The modeled temperature evolutions during the heating and cooling periods were also in accordance with the experimental and analytical data.
ACKNOWLEDGMENTS

This thesis presents the main results and analyses from numerical modeling studies executed at the University of Toronto during the past four years, under the supervision of Professor Paul Young. Before beginning my comprehensive research as a doctoral candidate at the University of Toronto, I was employed by a consulting engineering company specializing in high-level nuclear waste disposal research projects. While involved in one of the company’s international projects, I met my future supervisor Professor Paul Young. The project itself, a multinational collaboration, was a highly interesting underground heated in-situ experiment, and I had chance to be involved in running some exciting thermo-mechanical continuum simulations that were designed to predict the outcome of the experiment before it had actually started. My doctoral thesis also deals with thermo-mechanical modeling, but uses a discrete approach in comparing existing laboratory and field scale data against the modeled responses. During my work on this dissertation, three papers that are related to my ongoing research were published. Two of them are conference papers presented in international contexts. The third was submitted to a peer-reviewed journal and was published in July 2008 issue of the journal.

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LIST OF MAIN SYMBOLS AND NOTATIONS

AE/MS – acoustic emission, micro seismic
AECL - Atomic Energy of Canada Limited
APSE – Aspo Pillar Stability Experiment (Sweden)
DEM - Distinct-element method
FISH - Built-in programming language of PFC (and other Itasca codes)
HFT - heated failure test
Intergranular/intercluster – between grains/clusters
Intragranular/intracluster – inside a grain/cluster
LdB – Lac du Bonnet (granite)
PFC2D/PFC3D – Particle Flow Code in 2 and 3 Dimensions
TSX – Tunnel Sealing eXperiment (Canada)
URL – underground research laboratory

c – specific heat [J/kg K]
E - Young’s modulus [GPa]
K – thermal conductivity [W/m K]
UCS - Unconfined/uni-axial compressive strength, peak strength [MPa]
v - Poisson’s ratio
αt - thermal expansion coefficient [1/K].
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1 INTRODUCTION

The study of changes in the physical properties of rocks as a function of thermal cracking is a subject of widespread interest since it applies to human-induced applications such as the optimization of geothermal recovery, safe design of nuclear waste depositories (Figure 1-1), and also applies to natural processes such as volcanism and metamorphism. It is important to see how the perturbation of the environmental stress state caused by human activities may alter the rock structure, thus leading to changes in mechanical or transport properties of the host rock. Such alterations may have undesirable consequences on the integrity of the rock mass. The thesis presents the results and analysis of numerical simulations that were conducted in order to validate bonded-particle models for thermo-mechanical problems. Particle Flow Code (PFC) was chosen for the research because of its several benefits. The basic mechanical code has been available for the past ten years, and is being used mainly in primary research as well as in academic research. There is a diverse selection of published research using the code. However the thermal option is a more recent addition to the code and lacks extensive verification, validation and applications. The thesis is the answer for that.

The computer code is based on the original work by Cundall & Strack (1979). The code is classified as a discrete element method and it does not require pre-defined or initially imposed conditions for presenting damage during simulation. The code provides a natural heterogeneity of numerical specimens due to the random particle packing scheme. New particle clustering and grouping routines were developed and tested during the thesis work. The particle clusters were used to model the grain-scale effects in hard rock.
As a result of the explicit time marching calculation method, PFC exhibits dynamic material behavior where seismic waves propagate at a velocity dependent on the material properties. Data from an acoustic emission (AE) monitoring, a non-destructive testing method, can be readily compared with the synthetic seismicity of a PFC model.
Figure 1-1. In the concept of storing used nuclear fuel underground the canisters are placed in boreholes drilled from the deposition tunnels. Above- an artist’s view of the concept. Below – a tunnel in an underground research laboratory for used nuclear waste.
1.1 Validating numerical models

The purpose of the thesis’ main part is to build confidence regarding bonded-particle models for thermo-mechanical simulations. The section discusses the validation and possible usage of numerical tools in the modeling of physical systems. The following discussion is based on (Oreskes, Shrader-Frechette & Belitz, 1994) and (Starfield & Cundall, 1988), the latter of whom pay particular attention to rock mechanics.

In 1994, (Oreskes, Shrader-Frechette & Belitz, 1994) presented an analysis of the validation of numerical models. When constructing a model, we usually validate it in order to establish whether the model or code does indeed reflect the behavior of the real circumstances to which it refers. The most common method of validation is a comparison of measurements obtained from laboratory tests with the results obtained from computational models. It should be remembered, however, that agreement between measurements and the output of numerical modeling in no way demonstrates that the model that produced the output is an exact representation of the real system. When pursuing a good match, it must be remembered that more than one model construction can potentially produce the same output. Validation is thus a process of building confidence in models.

Numerical models are calibrated by manipulating independent variables. This is done with the aim of obtaining a match between the observed distributions of the dependent variables on the one hand, and the simulated distributions on the other. When more data becomes available that usually requires further adjustments. This complication has serious effects on the use of any calibrated model for predictive purposes, such as estimating the long-term stability of an underground opening.
Models can test mechanistic hypotheses by offering data that strengthens what may have already been partly established by laboratory tests. Models can therefore be considered as representations that are useful for guiding further study. The important reason for carrying out the modeling process is a lack of full access to the phenomena of interest.

(Starfield & Cundall, 1988) extend the discussion to the modeling of problems in the field of rock mechanics. The lack of detailed data in rock mechanics was a primary stumbling block in the early days of modeling, and the possibility of including additional data was eagerly welcomed. Later, the focus in rock mechanics moved from measurement to computation. Easy access to versatile, powerful, and inexpensive computer equipment has increased the extent to which models are employed. The computer tools themselves are not, however, an explicit solution, but rather a means to a solution. The following presents some key points as presented by (Starfield & Cundall, 1988); these points should be kept in mind when using modeling tools.

- A model is a simplification of reality. A modeling tool should be chosen for a specific task.
- The design of a model should be driven by the question that the model is expected to answer.
- Design the simplest possible model that will allow the mechanism being examined to occur.
- Implement the model, choose your simplest experiment, and conduct it. Once successful runs have been carried out, proceed to experiments that are more complex.
- Only run complex models once success has been achieved with simple ones.
- Visualize and anticipate solutions before actually running a model.

Modeling carried out in a cautious and considered manner leads either to new knowledge, or to an improved understanding of existing knowledge.

1.2 Objective of research

The main objective of the research presented in this thesis is to study, test, and validate thermo-mechanical bonded-particle models. The modeling method is based on the Particle Flow Code (Potyondy, Cundall & Lee, 1996), and uses bonded particles to represent hard rock (Potyondy & Cundall, 2004).

Validation is performed with the help of case studies, in which the modeled responses are quantitatively and qualitatively compared to the laboratory- and field-scale experimental data. This thesis also strongly focuses on the comparison of seismic-based results, and primarily uses data from acoustic emission (AE) as well as seismic velocity surveys. The former represents a sensitive method for studying crack locations, while the latter is an ideal method for quantifying changes in rock properties (Young et al, 2004).

1.3 Organization of thesis

The objective of Chapter Two (Previous work) is to show the current state of research in the area of thermal cracking in brittle materials, especially in hard rock. Chapter Three (Modeling method) describes the numerical methods used in the research work. The subsequent chapters include case studies in the laboratory scales (Chapter Four, Laboratory scale modeling) and field scales (Chapter Five, Field scale modeling). Each chapter includes
sections that discuss and explore the test results in the context of the validity of the applied models, as well as conclusive sections outlining concerns that require further study. The final chapter (Chapter 6, Conclusion) summarizes the key findings of the research work.
2 PREVIOUS WORK

An important practical application related to thermal cracking in brittle rocks is the concept of underground nuclear waste disposal. In this application, fuel canisters are placed in underground cavities. The disposed canisters produce residual heat that results from the decay of radioactive products. Heat spreads into the surrounding rock, causing a thermal gradient and a temperature increase in the surrounding rock volume. The resulting temperature increase might open existing microcracks or create new ones, which can coalesce to result in macroscopic fracturing. Eventually, this process may have unwanted side effects on the rock permeability around the disposal facility. There is thus an imperative demand for better preventive design methods that can be applied under extreme loading conditions and in the presence of cracks. The role of mechanical loading in fractures has been widely investigated. It is also of fundamental importance, however, to understand how thermal conditions affect crack growth and crack failure.

In what follows, a summary of laboratory-scale thermal experiments is given. This summary section considers the effects of temperature change on the material macro-properties of the affected rock, as well as on the micro-structural damage inflicted. After this, numerical modeling cases of thermally loaded rock are presented. These examples are divided up into cases that are related to underground nuclear waste and cases related to issues of deep reservoirs, and are accompanied with relevant analytical and micromechanical thermal studies.
2.1 Thermal experiments on rock

During the past years, the effects of temperature on the physical properties of rock have been widely studied. Experiments conducted on laboratory-scale specimens have shown that temperature does indeed affect the rock’s properties. Generally, the experiments had two main components: the effect of temperature on the macroscopic properties of rock, and studies on grain-scale effects, such as microcracking. Heuze (1983) compiled data on temperature-related properties of granitic rocks. Mechanical as well as physical properties (for example strength, modulus, cohesion, thermal expansion, specific heat, and thermal conductivity) were shown to be affected by high temperature, up to 1000°C, conditions. The data was based on numerous experiments that were conducted on granitic rocks prior to 1983, and that were aimed to be of immediate use to scientists involved in thermal modeling. Studies of changing rock properties in elevated temperatures have continued ever since.

The measured macroscopic properties, including static strength, deformability, and fracture toughness, tend to decrease with increasing temperature. This is known, for example, for marble and sandstone (Mahmutoglu, 1998), and for gabbro (Zhang et al, 2001). Heating-induced micro-structural damage can be detected by seismic velocity measurements, which have shown that due to microcracking, the measured seismic velocities tend to decrease with increasing temperature. Other velocity-related data like velocity anisotropy or wave attenuation are also used to study damage in rocks. Data gained in such experiments also showed that in initially isotropic samples, thermal cracking is roughly isotropic. This has emerged, for example, in experiments documented by David, Menendez & Darot (1999) who tested La Peyratte granite. Jackson, Lau & Annor (1999) observed the same decreasing
strength trend when testing Lac du Bonnet granite. Geraud et al. (1998) used a special triaxial cell in a X-ray tomography apparatus in order to observe porosity formation and macrocracking during heating and axial loading of granite samples. They also observed that heating induced porosity is homogeneously distributed throughout the sample.

Mahmutoglu (1998) conducted a study to open and loosen grain boundaries of rock specimen by cyclic heating and cooling. The tested samples were fine-grained rocks, Carrara marble, and Buchberger sandstone. The calcite that existed in the specimens used had anisotropic thermal expansion coefficients, and thus the potential to disturb the grain boundaries during heating cycles. The specimens were heated up to 600°C, then cooled down. Uniaxial compression tests were performed after the heating cycles for each specimen. The conducted tests showed clearly that with the increasing number of heating cycles, the compressive strength and the modulus of deformability drop. Furthermore, the amount of deformation at the peak strength level increased, which indicated the closing of grain boundaries loosened before by cyclic heating.

David, Menendez & Darot (1999) compared the effects of stress-induced cracking to those of thermal cracking. The rock type used was La Peyratte granite, which is generally described as fine grained, homogeneous, and with no crystal preferred orientations. The cored rock specimens were cracked by subjecting them to high temperatures (220°C and 450°C) or by loading them to high stresses (below ultimate strength) using a triaxial test apparatus. Once the specimens were cracked, several macroscopic properties were measured. The researchers concluded that the rock’s crack density increases with temperature, and that it affects several rock properties: porosity, seismic velocities, conductivity, and permeability. On the micro-
structural analysis, the researchers observed that the thermally induced cracks’ length increases more than the aperture, compared to those of the stress-induced cracks. On the other hand, Homand-Etienne & Houpert (1989) observed that with increasing thermal damage, crack aperture was enhanced without effecting significant variation in crack lengths.

Additional experimental studies of the detailed analysis of the thermal cracking in rocks were conducted by Davidge, (1981) and Menendez, David & Darot (1999). These studies concluded that thermal cracking is usually due to the mismatch in the thermal expansion coefficients between adjacent minerals, and produces randomly oriented grain boundary cracking. Cracking can also be due to the anisotropic nature of the thermal expansion coefficient.

According to Simmons & Cooper (1978), changes in temperature produce two kinds of cracks. Firstly, thermal gradient cracks formed due to the inhomogeneous strain produced by inhomogeneous temperature fields, and secondly, thermal cycling cracks formed due to the inhomogeneous strain of the mismatch of thermal expansion at mineral boundaries. The presence of cracks may modify the anisotropy of thermal expansion. The above-mentioned study on granite showed that the expansion anisotropy decreases with increasing temperature, and is most likely due to the formation of cracks that were more or less randomly oriented. The thermal expansion coefficient was smallest in the direction perpendicular to the plane of greatest crack concentration. Based on the experiments by de Castro Lima, Jose Janio & Paraguassu (2004), it was concluded that the thermal expansion coefficient is mostly affected by the rock’s porosity and is the same in all directions. The specimens were grouped according to their porosity, grain size, and quartz content, and then
related to linear thermal expansion coefficients. Grain size has only minor effects on the value of the thermal expansion coefficient. As the grain size decreases, the coefficient slightly increases. A 10% increase in quartz content increases the thermal expansion coefficient by about 20%. The experiments were conducted using cylindrical rock specimens cored in different directions. The expansion coefficients were measured in a temperature range of 0 to 50°C.

In 1974 Lindholm, Yeakley & Nagy performed laboratory experiments on Dresser basalt in order to study the strength of rocks under dynamic loading and in temperatures ranging up to 1200°C. The application the researchers were interested in was the improvement of drilling and fragmentation techniques. A series of high strain rate tests were performed on the cored cylindrical basalt specimens. The high impact velocities of the tests were achieved by using a pneumatically driven impact bar guided by a long launch tube. The high temperatures were generated with halogen lamps, and controlled with thermocouples mounted directly on the specimen. The energy required to induce fracture is related to the effective temperature. The energy input required to fracture basalt in compression increases with decreasing temperature and increasing strain rate. Since rock can be almost elastic to failure, the energy required to induce fracture is proportional to the strength.

Other dynamic studies on rock were conducted by Zhang et al. (2001). The cylindrical specimens of gabbro and marble samples were tested for dynamic fracture at high temperature. A V-shaped slot was cut at the upper edge of the specimens, where dynamic loading was then applied. The pre-heated specimens were loaded with impact bars, similarly to the tests performed by Lindholm, Yeakley & Nagy (1974), and fracture toughness values
were calculated. Fracture toughness describes the ability of rock to resist fracturing and the propagation of pre-existing cracks. Irrespective of the heating method used, it was noted that the rock’s ability to resist fracturing decreases with increasing temperature in static loading conditions. Test results indicated that fracture toughness increases with increasing loading rates, irrespective of the rock type. The influence of high temperatures on the dynamic fracture toughness, however, was quite limited. Observations of the fractured specimens with microscopes have shown that when the loading rate is very high, the branching cracks in a specimen penetrate the entire specimen, hence the formation of three or more fragments after fracturing. The high temperature produced micro-cavities inside the specimens even before loading. There were great numbers of such microcracks near the fracture surface, and they markedly increased the damage in the fracture surface.

The heating of rock creates microcracks which makes rock weaker and less stiff. This reduction in the values of the rock properties was observed in the presented experimental studies. It is therefore concluded that a change in the rock’s temperature is a factor influencing the characteristics of a rock.

2.2 Numerical thermal experiments

2.2.1 Experiments related to underground nuclear waste repositories

The impact of the heat generated by radioactive waste canisters on the stability of the repositories is one of the main concerns associated with underground waste disposal. In recent years, large-scale in-situ experimental and modeling studies have been conducted in
order to explore the effects of high temperatures on underground disposal facilities. An overview of the underground test facilities is given in (IAEA, 2001).

One of the first numerical studies was conducted by Liedtke & Kopiecz (1983). The researchers used a finite element method to model the effects of a cylindrical heat source on a rock mass. The numerical results were compared to the behavior of the actual in-situ experiment. In the experiment, a five-meter heater was placed in a vertical borehole and heated for a period of 150 days. During the experiments, temperature and displacements were monitored around the borehole. The material was modeled in accordance with a creep constitutive law. Possible failure areas were identified by interpreting stresses in the system and comparing those to an experimental effective-mean stress curve. If the modeled stress value was outside (above) the curve it was said that the modeling zone was failing.

Millard et al. (1995) summarize a thermo-mechanical modeling study on fractured rock mass that compared the results of four different modeling approaches. This work was part of an international research project called Decovalex.¹ The project studied various thermo-hydro-mechanical processes that are important for nuclear waste repositories. More recent summary of the studies was given by Tsang et al. (2005). In the work of Millard et al. (1995), the fractured rock mass was modeled either as an equivalent continuum, or each fracture was modeled individually. They summarize that the results from discrete approach experiments yielded a more accurate outcome, although no comparison to in-situ experiments was presented.

¹ Development of COupled models and their VALidation against EXperiments in nuclear waste isolation.
Another equivalent continuum study was performed by Min et al. (2005). Here, the researchers conducted a series of numerical experiments of fractured rock mass, using the distinct element method. By conducting mechanical and hydraulic tests at different loading conditions, a set of empirical rules was formulated. After this, the yielded material properties corresponding to different stress levels were passed to the large-scale finite-element code. Using the equivalent continua method, the results showed that the responses of fractured rock vary significantly based on how mechanical properties were determined. In intact rock masses, the thermal stress boost was very significant when compared to fractured rock, in which this concern had much less significance.

A more recent model comparison study, which was also part of the Decovalex project, was conducted by Rutqvist et al. (2005). Four research groups used different numerical models to simulate and predict coupled thermo-hydro-mechanical processes. The models used were continuum-based, with elastic or elasto-plastic constitutive material models. Modeling results of rock temperature, displacement, and fracture permeability were compared to measured responses from the in-situ Yucca Mountain Drift Scale Test (Wagner, Blair & Sobolik, 2000). The analyses modeled reasonable permeability responses; however, the modeled displacements tended to be not in agreement with the measured ones. Detailed description of the modeling approaches have been presented in (Hsiung, Chowdhury & Nataraja, 2005) and (Sonnenthal et al, 2005).

Guo et al. (2005) describe a numerical modeling study in the design of a full-scale heated tunnel experiment, which was conducted in an Underground Research Laboratory by
AECL.² Their model was continuum based as well, and studied the effects of heated fluid flows introduced to the system, also taking into account convection and conduction components. The modeling was carried out in order to assist the design of the experiment’s heating stage. Both during and after the experiment, the modeled temperatures at various locations were compared to the measured ones. It was found that the best temperature matches were occurring in the rock. In-floor waste placement in granitic rock and the subsequent temperature distribution around the facility was also studied by Sizgek (2005), who used a continuum finite volume method.

2.2.2 Experiments related to underground reservoirs

Modeling of thermal fracturing has important practical implications for fluid-injection wells in deep reservoirs. Clifford, Berry & Gu (1991) and Wang & Dusseault (2003) describe modeling and analytical approaches designed to estimate wellbore stability under thermal conditions. In the cases presented below, cooling of the rock and subsequent contraction reduces compressive stresses and introduces tensile fractures that affect the stability around the wellbores. The studies concentrated on calculating critical conditions, for example using Mohr-Coulomb criterion, for the stability using linear elastic models. Wang, Kassoy & Weidman (1987) developed a three-dimensional analytical model for temperature convection in a saturated fractured rock zone. Their application aim was the heat and mass transportation in geothermal systems that display vertical faults.

Another numerical model related to the cooling of rock is presented by Hicks et al. (1996). Their model simulated forced fluid flow through a fractured rock mass with accompanying extensive rock mass cooling. Here, thermal components were taken into account via stress changes that were based on the cooling of the rock and subsequent fracture openings in the cooled zones, which further affected the fluid flow in the system. In their experiments, rock mass was modeled as a linear elastic medium. Fracturing was represented as simplified orthogonal fracture sets. The goal was to investigate the effects of stress on the fluid flow. Similar studies on fractured warm reservoirs were conducted, for example, by Gutierrez & Makurat (1999), Henley & Hughes (2000) and Chen et al. (2003). The main concern in these studies was fluid-related, while thermal components were an additional factor that was seen as mainly affecting the fluid’s transportation properties. Shimizu (2006) developed a coupled particle thermal fluid scheme using PFC. In this approach, the thermal component involved convective and conduction heat transfers. The evolutions of the temperature fields were compared with analytical solutions. The results were in agreement under restricted conditions.

2.2.3 Thermal cracking studies

Keer, Nemat-Nasser & Oranratnachai (1979) analyzed the growth and interaction of parallel cracks at a solid’s free surface that was subjected to cooling. The work was relevant to the problem of heat extraction from hot dry rock masses. The analytical calculations of their experiments showed that the form of temperature profiles and crack interaction between adjacent cracks were the most important factor in the stability of the studied system. Cracks lengths were observed to increase, until a certain critical state was reached. Then, some
cracks stopped growing, whereas others continue to grow at a faster rate until a new critical state was reached. This process continues as the temperature front keeps penetrating the solid. This particular research approach was applicable to cases of the collinear extension of equally spaced edge cracks.

Walder & Hallet, (1985) presented another theory of the cracking of rock during cooling periods that used fracture mechanics principles. In their study, the driving force for the cracking was the growth of ice crystals in rock, rather than thermal contraction. Similar to the approach by Keer, Nemat-Nasser & Oranratnachai (1979), the study concentrated on crack growth as the temperature front penetrates deeper into material. However, cracks were found to be oriented randomly, and had penny-shaped forms (Keer was confined to linear parallel cracks). The simulated crack growth was achieved using material properties of Westerly granite and St. Pons marble. The researchers’ theoretical model indicated that the crack growth rate depended on a variety of material parameters, such as crack size, grain size, and grain shape. Another fracture mechanics approach was presented by Haddar, Fissolo & Maillot (2005), who studied thermal fatigue cracking in steel, and used the finite element method. The procedure included calculations of the propagation of a parallel crack network.

Giannopoulos & Anifantis (2005) analyzed frictional crack closure under thermal loading. They used a modified version of the boundary element method, in which the problem is divided into sub-regions, in order to be able to take the contact behavior of the crack surfaces into account. These were modeled as separate boundary surfaces with appropriate imposed conditions. The formulated two-dimensional analytical procedure was used to predict
frictional fracture interference in thermal loading. de Borst & Peeters (1989) used a smeared crack model to simulate the behavior of concrete under thermal loading. Their analytical approach was implemented using the finite element method, and took account of the temperature dependencies of the elastic properties and the effects of thermal dilatation. In the smeared crack model, the total strain was decomposed into crack-related and bulk material strains. The model was used to predict a fire test on a concrete slab. The method did not represent damage explicitly. A similar modeling approach was proposed by Pearce, Nielsen & Bicanici (2004).

Whittles, Kingman & Reddish (2003) discussed the fracturing of rock by microwave heating. They modeled heating-induced fracturing with the FLAC finite difference program (Itasca Consulting Group, Inc., 2002). The model consisted of two different mineral entities that were randomly positioned in the numerical sample. The model zones were heated according to the applied microwave heating. Actual fracturing was interpreted with a constitutive law, taking account of stresses and strains in model zones. By using a simple continuum model, it was shown that an increase of the microwave power (hence the applied temperature) results in higher stresses. Jones et al. (2005) conducted further sensitivity analyses on this problem, and studied, for example, the fact that the effects of different particle sizes showed that with smaller particles, more energy is needed to raise the temperature, and that thermal stresses are thus enough to damage the material. Wilson (2003) presented analytical models for rock failure that is due to thermal shock loading. He showed that internal cracking that results from a sudden increase of pore pressure can occur at only slightly elevated temperatures, unlike spalling (cracking at the material’s surface), which needed higher temperatures.
2.2.4 Micromechanical approaches in thermal modeling

In micromechanics, material microstructure is explicitly represented in computational models. Bruzzi & McHugh (2005) used a micromechanical unit cell modeling approach to study microstructural deformation in an aluminum alloy that had been subjected to a thermal treatment. In their work, the material showed microfractures that were induced by residual stresses due to the thermal expansion mismatch of the constituents. The numerical model was based on the finite element method, and the microstructure was represented as an idealized geometry. Damage was identified in plastic strain regions, but no damage mechanisms were included. In another case, the damage was allowed to occur by separating the nodes preceding the flaw along a predefined path. Hobbiebrunken et al. (2004) conducted a similar study on polymeric materials. Their model was constructed of fiber and composite parts, and based on the finite element method. The materials used were modeled as isotropic non-linear. Their model took into account the temperature dependencies of the input properties, such as the Young’s modulus, and the coefficient of the thermal expansion. A failure criterion was used to describe material strength. However, the model was not capable of producing fracturing directly. A different approach, documented by Schmitt et al. (2002), used modified thermal shock criteria for analyzing the thermal shock behavior of brittle ceramics, and was based on the finite element approach.

McHugh & Connolly (2003) studied crack propagation and ductile failure in metallic materials. They used a micromechanical approach, where the material ligaments were explicitly represented in the finite element model. The model was used to predict material behavior subjected to cooling from 1000°C to room temperature, a cooling effect that
produced residual stresses due to differences in the thermal expansion between the constituents. The damage was represented numerically, eliminating elements based on a predefined material damage parameter. For numerical reasons, elements were not completely eliminated, and small residual values of the element stiffness and stresses were retained. The study found that the modeled fracture toughness values were highly dependent on mesh resolution; finer meshes gave lower values. The same dependence on size was also observed using PFC2D to measure fracture toughness (Potyondy & Cundall, 2004).

2.3 Summary

The effect of temperature on rock properties has been studied widely. Experiments conducted on laboratory-scale specimens have shown that temperature clearly affects the rock’s properties. The experiments conducted consisted of two main components: firstly, analyses of the effect of temperature on macroscopic properties, and secondly studies on grain-scale effects such as microcracking. Thermal cracking has two initiation possibilities. Firstly, thermal gradient cracks that are formed due to the uneven strain produced by uneven temperature fields; and secondly, thermal cycling cracks that are formed due to the uneven strain resulting from the mismatch of thermal expansion at mineral boundaries. Analytical thermal cracking studies have shown that the crack growth rate is dependent on various material parameters including crack size, grain size, and grain shape.

The influence of the heat generated by radioactive waste canisters on the stability of underground repositories is one of the main concerns associated with underground disposal concepts of nuclear waste. Various modeling projects have studied the thermo-hydro-mechanical processes related to the underground disposal of nuclear waste. Most of the
models used in these studies were continuum based. The major concern in these studies has been the effect of the temperature on the fluid flow in the analyzed systems, as well as the temperature distribution around the displaced fuel canisters. Another field of inquiry related to thermal modeling is the analytical focus on underground reservoirs. Here, studies have concentrated on the stability around wellbores subjected to thermal changes in the host rock, and on the simulations of fluid flows through fractured rock mass as well as accompanying thermal effects. In micromechanical approaches, the material’s microstructure was explicitly represented in computational models. In these models, thermal effects were integrated with the corresponding failure criteria, which were used to describe the material strength. Other approaches that represented the damage by numerically eliminating model elements, were based on predefined material damage parameters.

In previous studies of numerical approaches relating to thermal fracturing of hard rock, the models used have mainly been continuum-based and the damage predictions enabled by these models were carried out indirectly by interpreting, for example, the strength of the rock in question based on stresses calculated in the model. Approaches designed to quantify thermal damage of brittle rocks have lacked the ability to produce spontaneous cracking behavior. Cracks were either previously introduced to the material, or they propagated via a prescribed path. A discontinuum particle model is therefore proposed for the modeling of the complex features of the failure processes. In this research, the heating-induced cracks initiate spontaneously, and then propagate based on the system state, producing at any moment a behavior comparable to the observations of both the laboratory and in-situ scale experiments.
3 MODELING METHOD

The research conducted in this thesis made extensive use of a commercially available modeling tool called Particle Flow Code in 2D (PFC2D), as well as the 3D version PFC3D. There are some other codes, such as Y2D (Munjiza. 2004) and Fracod (Bäckström et al. 2008), which are capable of producing cracking but at the moment they lack the thermal routines, and furthermore do not have a wide user base. The research concentrated on thermal problems related to hard rock. In the following sections, a summary of the code used for the modeling is given; this is followed by a description of the thermal formulations in the PFC software. In the analysis of the simulation results, seismic methods such as acoustic emission (AE) monitoring were used, which will be described in more detail in the subsequent section. Some of the numerical specimens were created with particle clusters. This method is described in the last section of the chapter.

The files to run the presented simulation cases are included in the accompanying disk.

3.1 Particle flow code, PFC

PFC2D and PFC3D were used in the modeling of the thermal experiments. This approach simulates the movement and interaction of circular (2D) or spherical (3D) particles following the distinct element method introduced by Cundall (1971). The mechanical behavior of the system is described by the movement of each particle and the force and moment acting at each contact. Newton’s second law is used to determine the translational and rotational motion of each particle arising from the contact forces, applied forces and body forces acting upon it, while the force–displacement law is used to update the contact forces arising from the relative motion at each contact. The dynamic behavior is represented numerically by a
time stepping routine in which the velocities and accelerations are assumed constant within each time step. The solution scheme is identical to that used by the explicit finite-difference method for continuum analysis.

Solid rock is represented by an assembly of particles that are joined together by breakable parallel bonds, hence the name bonded-particle model. A parallel bond approximates the mechanical behavior of brittle elastic cement joining the two bonded particles. Parallel bonds establish an elastic interaction between these particles that acts in parallel with the grain-based portion of the force–displacement behavior. The bonds can transmit both forces and moments between particles. If the maximum stress exceeds the set strength, tensile or shear, then the parallel bond breaks and it is removed from the model along with its accompanying force, moment and stiffnesses. The damage, thus, occurs by bond breakages, and the studied material transforms from solid to granular. Another bond type available in PFC is called contact bond which is a simplified form of bonding. A contact bond approximates the physical behavior of a vanishingly small cement-like material lying between and joining the two bonded particles. A contact bond does not have a radius or shear and normal stiffnesses, as does a parallel bond, and cannot resist a bending moment; it can only resist a force acting at the contact point. The detailed description of the PFC2D model for rock is given in Potyondy & Cundall (2004).

Based on earlier studies, the PFC modeling method has some known deficiencies that were summarized for example in (Potyondy & Cundall, 2004). One of the key issues is the inability to match both compressive and tensile strengths in a single PFC material. The measured macroscopic strength can be calibrated to either UCS or Brazilian tensile strength,
but not both simultaneously. The ratio of the UCS to tensile strength seems to be about five for a PFC material. The ratio value for a brittle hard rock is closer to 20. PFC material also underestimates the slope of the strength envelope as a function of confining stress. Potyondy and Cundall (2004) further hypothesized that the issues could be reduced by using grain shapes that more closely resemble the complex-shaped and highly interlocked crystalline grains in granite. In addition, the correspondence between particle size and the material’s mechanical properties plays a major role in PFC modeling. It is an intrinsic part of the material characterization and cannot be regarded as a free parameter that only controls model resolution.

PFC2D has been used to simulate, for example, hydraulic fracturing (Al-busaidi, 2004), seismic velocities (Hazzard & Young, 2004), failure around a circular opening (Fakhimi et al, 2002), crack initiation and interaction in hard rock (Diederichs et al, 2004, Diederichs, 2003) as well as its impact on tunnel liner (Wang & Tannant, 2004). Dedecker, Billaux & Gentier (2003) used the approach to model heat flow near a borehole. In their study, a preexisting fracture was included in the model, as well as simulated hydraulic pressure. The model reproduced physical phenomena observed in-situ, although no direct comparison was made.

3.2 Thermal formulation in PFC

Conduction of heat means that the heat passes through the substance of the material body itself (Carslaw & Jaeger, 1965). The general formulation for heat flow across any material is given by Equation 3-1.
\[ pC \frac{dT}{dt} + \left( \frac{df_x}{dx} + \frac{df_y}{dy} + \frac{df_z}{dz} \right) = 0, \]

where \( T \) is temperature, \( t \) is time, \( C \) is specific heat, \( \rho \) is density, and \( f_x, f_y \) and \( f_z \) are the heat fluxes in three coordinate directions. The formula is valid at any location in the material. In a homogeneous isotropic solid, the thermal conductivity \( (K) \) is independent of temperature, and therefore fluxes are given by Equation 3-2.

\[
f_x = -K \frac{dT}{dx}, \quad f_y = -K \frac{dT}{dy}, \quad f_z = -K \frac{dT}{dz}
\]

When Equation 3-2 is inserted into Equation 3-1, the equation of heat conduction simplifies to Equation 3-3.

\[
\nabla^2 T = \frac{\rho C}{K} \frac{dT}{dt}
\]

The first thermal PFC2D thermal problem is presented in Chapter 4, and deals with a temperature difference between outer and inner regions of a rock cylinder. An analytical temperature profile for steady-state hollow cylinders (Carslaw & Jaeger, 1965) was derived using cylindrical coordinates, and is given by Equation 3-4.

\[
T(r) = \frac{T_a \ln\left(\frac{b}{r}\right) + T_b \ln\left(\frac{r}{a}\right)}{\ln\left(\frac{b}{a}\right)}
\]

where \( a \) and \( b \) are inner and outer radii of the cylinder, respectively, and \( r \) is the radial distance from the origin.
Based on thermoelastic theory (Portu, 1992), an analytical solution for a critical temperature difference across a cylinder for a tensile failure is calculated, and presented by Equation 3-5. The cylinder is an infinitely long and hollow concentric shape experiencing radially moving outward heat flow.

\[
\Delta T_{\text{critical}} = \tau \frac{1 - \nu}{E \alpha_t} \left[ \frac{2 \ln \left( \frac{a}{b} \right)}{1 - \frac{2a^2}{b^2 - a^2} \ln \left( \frac{b}{a} \right)} \right]
\]

where \( E \) is Young’s modulus, \( \nu \) is Poisson’s ratio, \( a \) and \( b \) are the inner and outer radii of the cylinder, \( \alpha_t \) is the thermal expansion coefficient, and \( \tau \) is the tensile strength of the material. When working with average granitic rock properties, the calculated critical temperature difference (for failure) of a cylinder with the inner and outer radii of 15 mm and 150 mm, respectively, is about 60°C. This analytical approach demonstrates that theoretically, the failure can occur easily even with a modest temperature difference for brittle materials.

Thermal algorithms in PFC allow the simulation of heat conduction and the development of thermally induced displacement and forces. In these algorithms, thermal material is presented as a network of heat reservoirs (particles) and thermal pipes (contacts between particles). Heat flow occurs via conduction in the pipes connecting the reservoirs. This approach allows the evolution of the heat network during the modeling. An overview of the thermal algorithms is given below, and the comprehensive description is provided in (Itasca Consulting Group, Inc, 2004b).
Each reservoir (model particle) is associated with a temperature \((T)\), a mass \((m)\), a volume \((V)\), a specific heat \((C)\), and a linear thermal expansion coefficient \((\alpha)\). A pipe, which connects two reservoirs, is associated with a power \((Q)\) and a thermal resistance \((\eta)\). Each pipe is regarded as a one-dimensional line with a length of \(L\); the power in a pipe is given by Equation 3-6.

\[
Q = -\frac{\Delta T}{\eta L}, \tag{3-6}
\]

where \(\Delta T\) is the temperature difference between the two connecting reservoirs at each end of the pipe. A heat conduction equation for a single reservoir is given by Equation 3-7.

\[
-\sum_{p=1}^{N} Q + Q_{v} = mC \frac{\partial T}{\partial t}, \tag{3-7}
\]

where \(Q_{v}\) is a possible heat source, and the summation represents the power in pipes that are aligned towards the exterior of the reservoir.

The thermal input parameters for a thermal PFC model are the specific heat \((C)\), the linear thermal expansion coefficient \((\alpha)\), and the thermal conductivity \((K)\). In PFC, the conductivity tensor is estimated for a given material; then, the thermal resistance computed from the conductivity is assigned to all pipes. This approach produces a thermally homogeneous material with a given macroscopic conductivity. The thermal resistance in terms of conductivity \((K)\), an area of interest \((A)\), and a length of thermal pipe (a line which connects the centroids of the particles in contact) over the area \((l)\) is given by Equation 3-8.
In this equation, the summation adds the lengths of all the pipes situated in the area of interest. The heat conduction only occurs between particles that are in contact. It should be noted that new contacts could form anytime during a simulation, even between particles that were separated earlier by a bond breakage.

Temperature changes in a model produce thermal strains via thermal expansion. This is accounted for by changing particle radii and modifying bond forces. Particle radii are modified based on $\alpha_t$ and temperature changes on each particle. Each bond between two particles is carrying both normal and shear components of the force. Thermal expansion is accounted for the normal component of the force vector ($\bar{F}^n$) by effectively changing the bond length with Equation 3-9. This approach gives a force increment due to the thermal expansion, which is added to the current value of the force vector. When the temperature change is negative, the normal force in a parallel bond increases, and vice versa.

$$\Delta F^n = -\bar{k}^n A \alpha_t L \Delta T,$$

where $\bar{k}^n$ is the parallel bond normal stiffness, A is the area of the parallel bond cross section, and L is the bond length.

The thermal formulation for a heat flow was tested and compared to the analytical solution for a steady-state temperature profile. Two PFC specimens – a two dimensional circular (with PFC2D) and a three dimensional cylinder (with PFC3D) – were constructed with about 5000 and 70000 particles, respectively. The diameter of the specimens was 300 mm, with an
inner borehole diameter of 30 mm. The height of the PFC3D specimen was 220 mm. The perimeter surface temperature was set to 20°C, and the inner heater was set to 160°C. The model was cycled until steady-state conditions were met. The corresponding analytical steady-state temperature profile for a hollow 3D cylinder was calculated using Equation 3-4. The simulated and analytical temperature profiles are shown in Figure 3-1. The correlation of the profiles is convincing.

Figure 3-1. Comparison of PFC2D and PFC3D models and analytical temperature profiles across a cylinder subjected to inner and outer temperatures of 160°C and 20°C, respectively.
3.3 Acoustic emission and seismic waves in PFC

PFC uses an explicit time-marching calculation scheme to simulate the material behavior. This allows dynamic simulations to be performed, in which seismic waves propagate across the material at a speed that depends on material properties (such as stiffness of the particle contacts). During the simulations, each bond breakage is assumed to be a microcrack. When a bond breaks, the stored strain energy is released as kinetic energy in the form of a seismic wave. Microcracks that occur close together, both in space and time, are considered a single seismic AE event. The time in which the second microcrack needs to form in order to be included in the AE event is determined by the shear wave speed of the material. Therefore, if a second microcrack forms within the source area (particles in contact with the active one) and within the defined time period, the crack is considered part of the same AE event. Furthermore, a fast propagating fracture across the numerical specimen would be considered as a single AE event. When a crack occurs, the forces will be integrated around the crack by observing all contacts of the two balls on either side of the crack. The moment tensor will be calculated each time step and the magnitude will be calculated from the elements of the moment tensor matrix. The magnitude of the event will be the maximum observed over the event duration. This approach permits realistic event magnitude distribution and source mechanism results, and is based on the work of Hazzard & Young (2002). Pressure (P) wave velocities in a random particle assembly can be measured by propagating displacement waves through the material, and by monitoring the particle movement at a certain distance from the source. The wave velocity is calculated by determining the time difference of the peaks of the source and received waveforms. The wave velocity is related to the stiffness of the system. The stiffness of a PFC material decreases when cracks form and this can be
detected by measuring the velocity changes. Details on the numerical seismic monitoring technique are given in Young, Hazzard & Pettitt (2000), Hazzard & Young (2004), Hazzard & Young (2004), and Hazzard (1998). The source type classification of the AE events in the heated cylinder simulations (Section 4.1) was done based on the moment tensor isotropic component (k). If k was > 0.2, the event was classified as tensile, if k is <-0.2, it was compressive, and otherwise it was classified as a shear event (Pettitt, 1998).

3.4 Clustering PFC particles

A particle cluster is defined as a set of pre-defined number of particles that are in contact with each other. The use of PFC particle clusters is a relatively new concept that is becoming more feasible due to increasing computer power. It is also becoming more popular because of the ways in which it more closely matches the microstructure of complex materials such as rock. Cho, Martin & Sego (2007) showed that rigid particle clusters (called clumps) could be used to reduce some of the deficiencies in the particle-based modeling studies, such as matching the failure envelope.

There are few other studies on cluster size and its effect on the macroscopic behavior of the PFC material. Boutt & McPherson (2002) used PFC2D and studied the effect of varying cluster sizes (two to three particles) and the intercluster strengths to simulate the failure envelopes and damage types in a sedimentary rock. The clustered material seemed to increase the slope of the strength envelope (i.e. strength plotted against confining pressure) of a triaxial compression tests. Similar observations were made by Potyondy & Cundall (2004) who used unbreakable bonds and concluded, when comparing the strength envelopes to that of LdB granite, that the best fit was using cluster size of five particles in PFC2D. The
reason for the increase in the slope envelope is attributed to the complex shapes which under
an increasing confinement resist the movement past each other and thus increase the overall
compressive strength.

Landry, Lague & Roberge (2006) used PFC3D to model manure products in an agriculture-
related problem. Clusters were introduced to better model the friable and clumpy nature of
organic fertilizers. The researchers developed their own clustering routines and generated
materials with clusters of three or six particles. The clustered PFC3D material was tested
using a direct shear test. In the study, they varied modulus values, stiffness ratios, friction
coefficients, bond strengths, and contact models. The results showed connections between
the varied parameters and the measured angle of the internal friction (i.e. the slope of the
clusters to model rockfill dams. The differently shaped clusters were used to study the
stability of the dam. The researchers concluded that for loose unbonded materials, particle
packing is an important factor.

In the research presented in this thesis, the particle clusters were used to represent the
mineral grains in the thermo-mechanical PFC3D modeling simulations. The simulation
results using the PFC3D specimens are presented in Chapter 4. For the purpose of this study,
the existing clustering routines were enhanced to allow multiple clusters to be identified and
subsequently grouped. The development of the cluster routines is described below.

The clustering routine provided with PFC is described briefly in (Potyondy & Cundall,
2004), and can be summarized as follows. The routine starts with a densely packed bonded
PFC specimen, and then identifies the particle clusters. The routine is controlled by one
parameter, $S$, which is the maximum number of particles in a single cluster. There is no control over the cluster shape. The contacts, or bonds, are distinguished as intracluster bonds (between particles inside a cluster) and intercluster bonds (between particles in different clusters). This allows the setting of different properties for these two entities. There is, however, no distinction between different clusters. This additional functionality was developed, tested and ultimately applied during the thesis work. After which, it was possible to introduce collections of different clusters, called cluster groups, (like minerals in rock), and to assign different properties to different clusters. Figure 3-2 visualizes the progression of a regular PFC2D specimen to a specimen with cluster groups.

The developed numerical routine starts with a clustered PFC specimen in which each cluster is identified by a unique ID number that is stored with the other particle data. The routine fills a numerical array with the cluster IDs. The routine then shuffles the IDs to a random order. This procedure is similar to shuffling playing cards, where a single card is taken from a card pile and then placed to another random location before taking the next card. The size of the array (card deck) does not change during the shuffling. The array of randomly ordered cluster IDs is then sub-divided into a given number of groups by a subsequent routine: loop through all the particles in the PFC specimen, retrieve the corresponding cluster ID, match with the cluster group, and assign the group with the current particle. Following the cluster grouping routine, it is possible to assign different thermal and mechanical properties to different particle cluster groups in addition to applying different properties inside and between the groups. This enables studies of the thermal damage evolution with respect to grain boundary cracking. The thermal expansion contrast between adjacent clusters was the hypothesis of the thermal damage in the clustered PFC material.
Figure 3-2. Left pane – Cluster grouping routine. Right pane – top: a regular PFC2D specimen, middle: clustered specimen, bottom: clusters are grouped to two groups.
4 LABORATORY SCALE MODELING

Two laboratory scale modeling case studies were carried out. The first concentrated on induced synthetic acoustic events (AE) that were due to the thermal loading, while the second case focused on the wave velocity changes in the numerical specimen, which were due to increased damage during the heating. Both studies were based on existing laboratory data from previously conducted and published experiments. The modeled responses are compared with the laboratory data, and similarities and differences are highlighted in order to assess the validity of the thermo-mechanical models.

The first study is based on an existing laboratory experiment by Jansen et al (1993). Using a heater cartridge that was placed into a central borehole they heated a cylinder of Lac du Bonnet granite (LdB). AE monitoring during the experiment showed the development of the cracking in the specimen enabling an analysis of the temporal and spatial evolution of the heat-induced damage. Because of the high tensile hoop stresses produced by a strong thermal gradient, the rock sample ultimately failed. In the modeling study, the experiment was repeated using PFC2D and the laboratory data was then qualitatively compared to the response of the numerical model.

The second numerical study describes steps taken to implement and test the enhanced particle clustering routines in PFC. Here, numerical specimens replicated the properties of Westerly granite. In the simulations, PFC3D cubic specimens were heated up to 450°C. During the heat-induced cracking, AE activity and temperature evolutions were monitored. P wave velocity measurements were conducted for each of the numerical specimens. The
responses were compared with similar thermal laboratory data by Nasseri, Schubnel & Young (2007).

4.1 Heated cylinder experiment

4.1.1 Experimental data

Existing laboratory experiment data was used to validate the numerical model response. With a heater placed in a central vertical borehole, a sample of LdB pink granite was thermally cycled to progressively higher peak temperatures. Six heating cycles were performed, with peak temperatures ranging from 75°C to 245°C. A detailed description of the experiment is given in (Jansen et al, 1993) and (Carlson, Jansen & Young, 1993). The rock sample was obtained from Underground Research Laboratory (URL) located in Pinawa, Manitoba, Canada. It was a 30 cm diameter and 22 cm long cylinder with an axial borehole of diameter 3 cm penetrating the entire length of the sample (Figure 4-1). Using an array of transducers distributed around the sample, seismic data was collected during the heating and cooling phases. Source locations were calculated using an iterative fitting method, and mechanisms for picked events were generated using the polarities of the first arrivals. Events were then categorized as tensile, compressive, complex, and unknown.
Figure 4-1. The LdB granite specimen during the heating experiment. The array of AE transducers bounds the specimen.

In the first two thermal cycles, only a few AE events were detected. The events were located around the inner borehole (i.e. near the heater), and were mostly shear. Later pre-failure events, mainly tensile, were sparsely distributed throughout the sample (Figure 4-2, left side). During the final thermal cycle, the events started to localize along the would-be failure plane. After the failure, events occurred along the fracture face, as seen in Figure 4-2, right side. These failures were due to the shearing of the failure planes against each other. Equal amounts of compressive and shear events were detected in the post-failure phase. The dominant AE concentration corresponded with the visual observations of the fracture.

The results were interpreted to signify that the fracture plane initiated at the outer surface of the sample, and then propagated inward toward the heater. The major fracture was driven by
a strong thermal gradient that generated tensile hoop stresses in the cooler outer portions of the sample. Portu (1992) illustrates a similar phenomenon with the following explanation:

For a material subjected to a temperature difference from a higher inner temperature to a lower outer one, the surface layers cool faster than the inner material. Because the core prevents outer surface layers from contracting freely, they are subjected to tensile stresses. The inner zones, on the other hand, are under a compressive state. Since the tensile strength of brittle materials such as rock is one order magnitude lower than their compressive strength, fracture initiates at the outer surface.

Figure 4-2. Pre-failure (left) and post-failure (right) AE events of the laboratory sample. AE source types: diamond – shear, square – tensile, cross – compressive, triangle – complex, plus – unknown. (Carlson, Jansen & Young, 1993).
4.1.2 PFC2D Numerical models

The laboratory experiment was simulated with PFC2D software, since the laboratory cylinder was relatively long and could therefore be modeled realistically in 2D. The numerical specimens for LdB granite were based on the strength and deformation properties defined by Martin (1993) and presented in Table 4-1. The specimens were parallel-bonded, and were created using the well-established material genesis procedures described for example in (Potyondy & Cundall, 2004). Uniaxial and Brazilian tests were performed on the numerical specimens in order to determine their macroscopic properties. The macroscopic deformation and strength properties of the numerical specimens, labeled mA, mB, and mC, as well as of the actual LdB granite are given in Table 4-1. The main difference between the numerical specimens was the strength. The number of particles in each of the specimens was about 11,000. For LdB granite, the value of the thermal expansion coefficient $\alpha_t$ was found to be between $3.2 \times 10^{-6}$ K$^{-1}$ and $15.8 \times 10^{-6}$ K$^{-1}$ (Baumgartner et al, 1996) and (Jackson, Lau & Annor, 1999). Because these values vary to a certain degree, several numerical specimens with varying $\alpha_t$ values were created.

In addition to varying $\alpha_t$, two different thermal material types (homogeneous and heterogeneous) were introduced. These differed in the way the values of $\alpha_t$ were assigned to model particles. In the homogeneous thermal material, the same value of $\alpha_t$ was associated with all the model particles. In the heterogeneous material, three different particle sets, replicating quartz, plagioclase and biotite minerals, were identified in the specimen. Based on this, three different thermal expansion coefficients were assigned for those particles. The expansion coefficient values for the particle groups were adopted from (Fei, 1995), who lists
expansion coefficients for rock-forming minerals. The particles belonging to each set were scattered randomly throughout the specimens. The amount of particles in each of the mineral set approximated the fraction of that mineral in LdB granite; quartz particles 30%, plagioclase 40%, and 30% biotite particles. Figure 4-3 shows the two material types; homogeneous and heterogeneous (with three distinct sets of particles). The idea behind the described approach was to study whether cracking occurs between particles of the same expansion coefficient, or between particles with different coefficients (i.e. due to a difference in the thermal expansion). The hypothesis was that due to the experimental geometry, the strong thermal gradient overcomes the anisotropy effect, and the two different thermal models produce similar results. Thermal input properties of the models are shown in Table 4-2 from (Itasca Consulting Group, Inc, 2004b) and (Fei, 1995).

The heater was modeled by identifying a set of particles situated around the central borehole, and was designed to control the temperature of those particles during the modeling. The heating routine gradually raised the temperature of the heater particles. In between heating steps, the model system was cycled to mechanical equilibrium. The undulating temperature graph (seen for example in Figure 4-5) is an artifact of the numerical heating routine. The temperature of the outer particles was fixed to 20°C, simulating room temperature. The fixing of the temperature of the outer particles slightly boosted the temperature gradient effect. More realistic boundary conditions would also take into account convection and radiative boundary properties between the specimen and the surrounding air. However, these were considered of secondary importance, and were not incorporated in this study. Figure 4-4 shows the model set-up with heater particles and outer boundary particles identified by
arrows. During the simulations, temperature was measured at four locations, as marked in Figure 4-4.

The numerical specimens were combinations of assigned mechanical and thermal properties. For example, specimen ‘mB_tE’ had mechanical properties, coded mB from Table 4-1, and thermal properties of tE from Table 4-2. A total of about 15 combinations, i.e. different specimens, were tested. Computer simulation time varied from 25 to 100 hours per model, using a PC with a processing speed of a 3.0 GHz.
Table 4.1. Mechanical properties of PFC2D specimens and LdB granite.

<table>
<thead>
<tr>
<th>Mechanical model</th>
<th>mA</th>
<th>mB</th>
<th>mC</th>
<th>granite</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Microproperties (Input)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mean grain diameter [mm]</td>
<td>2.6</td>
<td>2.6</td>
<td>2.6</td>
<td>3</td>
</tr>
<tr>
<td>Mean bond strength [MPa]</td>
<td>157</td>
<td>94</td>
<td>32</td>
<td>-</td>
</tr>
<tr>
<td>Bond and contact modulus [GPa]</td>
<td>62</td>
<td>62</td>
<td>62</td>
<td>-</td>
</tr>
<tr>
<td>Particle density [kg/m3]</td>
<td>3170</td>
<td>3170</td>
<td>3170</td>
<td>-</td>
</tr>
<tr>
<td><strong>Macroproperties (Output)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Compressive uniaxial strength [MPa]</td>
<td>199</td>
<td>150*</td>
<td>50*</td>
<td>200</td>
</tr>
<tr>
<td>Young’s modulus [GPa]</td>
<td>67</td>
<td>67*</td>
<td>67*</td>
<td>69</td>
</tr>
<tr>
<td>Tensile strength from Brazilian test [MPa]</td>
<td>46</td>
<td>28</td>
<td>10</td>
<td>9.3</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.32</td>
<td>0.32*</td>
<td>0.32*</td>
<td>0.25</td>
</tr>
</tbody>
</table>

* Estimated values based on the UCS/tensile ratio (5), elastic constant are generally not dependent on strength
+ Normal and shear bond strengths were set to equal values to reduce the number of free parameters.

Table 4.2. Thermal input properties of the material (Itasca Consulting Group, Inc, 2004b).

<table>
<thead>
<tr>
<th>Thermal model</th>
<th>tD</th>
<th>tE</th>
<th>tF</th>
<th>tG</th>
<th>tH</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bulk density [kg/m3]</strong></td>
<td>2650</td>
<td>2650</td>
<td>2650</td>
<td>2650</td>
<td>2650</td>
</tr>
<tr>
<td><strong>Specific heat [J/kg K]</strong></td>
<td>1015</td>
<td>1015</td>
<td>1015</td>
<td>1015</td>
<td>1015</td>
</tr>
<tr>
<td><strong>Thermal conductivity [W/m K]</strong></td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
</tr>
<tr>
<td><strong>Thermal expansion coefficient [1/K]</strong></td>
<td>3.5 x10^-6</td>
<td>15 x10^-6</td>
<td>10.0 x10^-6</td>
<td>16.5 x10^-6</td>
<td>9 x10^-6</td>
</tr>
</tbody>
</table>

* tD, tF and tG – homogeneous thermal material, tE and tH – heterogeneous thermal material
Figure 4-3. Above - homogeneous and heterogeneous thermal materials. The particles belonging to different sets are identified with different shades in the heterogeneous material. The dark particles belong to the heater element. The dark lines depict the forces in the bonds; width of the line depicts magnitudes. Below – force distribution in the bonds between particles shows that the forces vary more in heterogeneous material.
4.1.3 PFC2D Simulation response

The numerical heating simulations, as explained in the previous section, mimic the laboratory thermal experiment, where the temperature was gradually increased during six thermal loading cycles. During the heating, spatially scattered cracking is observed to occur in an increasing manner with increasing temperature. At some point, the temperature reaches a value at which the thermally induced stresses exceed the material’s strength, and failure occurs. This point is defined as the temperature at which a rapid increase in microcracking occurs. In the PFC2D material, this value was found to depend mainly on the value of thermal expansion and on the material strength. Increasing the thermal expansion coefficient reduced the failure temperature, while an increase in the material strength raised the failure
temperature. Between different PFC2D models, the failure temperature varied between about 120°C and 300°C, Table 4-3.

Table 4-3. Failure temperatures for various PFC2D modeling cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>Failure temperature [°C]</th>
<th>Thermal material type</th>
<th>Tensile strength [MPa]</th>
<th>Mean thermal expansion</th>
</tr>
</thead>
<tbody>
<tr>
<td>mA_tE</td>
<td>320</td>
<td>heterogeneous</td>
<td>46</td>
<td>16.5</td>
</tr>
<tr>
<td>mB_tE</td>
<td>160</td>
<td>heterogeneous</td>
<td>28</td>
<td>16.5</td>
</tr>
<tr>
<td>mB_tG</td>
<td>180</td>
<td>homogeneous</td>
<td>28</td>
<td>16.5</td>
</tr>
<tr>
<td>mC_tD</td>
<td>290</td>
<td>homogeneous</td>
<td>10</td>
<td>3.5</td>
</tr>
<tr>
<td>mC_tE</td>
<td>60</td>
<td>heterogeneous</td>
<td>10</td>
<td>16.5</td>
</tr>
<tr>
<td>mC_tF</td>
<td>115*</td>
<td>homogeneous</td>
<td>10</td>
<td>10.0</td>
</tr>
<tr>
<td>mC_tG</td>
<td>60-80*</td>
<td>homogeneous</td>
<td>10</td>
<td>16.5</td>
</tr>
<tr>
<td>mC_tH</td>
<td>110*</td>
<td>heterogeneous</td>
<td>10</td>
<td>16.5</td>
</tr>
</tbody>
</table>

* no actual failure due to extreme borehole damage.

4.1.4 Comparison with laboratory data

During the heating phase, the cracking in the models slightly increased until the temperature reached a critical value, after which the cracking started to increase more rapidly, and finally led to the specimen’s failure. Figure 4-5 shows the temperature histories and microcracking amount for three PFC2D modeling cases, as well as the AE count from the final (sixth) thermal cycle of the laboratory experiment. Model mB_tE failed at about 160°C. Model mA_tE did not fail at the first set temperature. The specimen was therefore exposed to additional heating to a higher temperature, and failed at about 300°C. The model mC_tF, on the other hand, failed at a lower temperature, before the temperature reached its first set maximum value of 250°C.
The development of the macroscopic failure is shown in Figure 4-6 (upper). In this model, the final failure initiated from the outer surface of the specimens, and propagated inward. The driving force for the failure was strong tangential stress at the specimens’ outer boundary. This was verified by observing the forces in the model’s bonds, as shown in Figure 4-6 (lower). This showed that there were significant tensile forces at the model boundary. The bonds near the borehole, on the other hand, were in compression. Similar tensile stress-driven failure was observed during the laboratory experiment of the heated cylinder.
Figure 4-5. Temperature, normalized AE activity in the laboratory experiment (upper left hand plot), and normalized cracking in 3 modeling cases during heating. The slightly undulating temperature curve is caused by the numerical heating routine.
Figure 4-6. The fracture propagates (arrows point to the crack tip) from the outer surface of the model mC_tF (left – timestep 52813, right – timestep 52816). Lower plot depicts forces acting in the model, black-tensile at the boundary and gray-compression in the middle.
The failure of the models depended mainly on the strength and thermal expansion coefficients of the particles. The assigned bond strengths have a direct impact on the failure temperature. The weaker the material, the lower the temperature at which the specimen fails. Decreasing the material thermal expansion coefficient, on the other hand, yields a higher failure temperature, even though the base material itself is not stronger.

In some modeling cases (for example case mC_tG), the local stresses in the vicinity of the borehole exceeded the strength of the material, producing major cracking at the borehole walls. This happened before the temperature difference between the borehole and outer boundary grew (due to thermal conduction) enough to produce high tensile stresses at the boundary. Cracking at the borehole wall was produced by high compressional stresses. In some other modeling cases, major cracking occurred near the borehole, while the main failure was still along a fracture plane initiating from the outer surface. The cracking at the borehole wall also affected the heating of the specimen. When borehole cracking occurred, some of the heater particles detached from the borehole wall, disabling heating at some portions of the specimen, thus affecting the overall temperature field.

The macroscopic failure behavior between the numerical simulations and the laboratory experiment are very similar. In both cases the failure began from the outer surface which was interpreted to be due to high tensile tangential stresses. A few differences were also observed. During the laboratory experiment, scattered cracking occurred during both the heating and cooling phases. In the numerical simulations, cracks only formed during the heating phases. The microstructure of the model is considered to be too simple to produce cracking during cooling. More complex particle clusters could be introduced in order to
produce contraction cracking during cooling. It was hypothesized that more complex particle shapes would allow stresses to be locked during the thermal cycling that then could lead to additional cracking when the specimen is cooled.

By definition, a parallel bond fails when the stress in the bond exceeds the assigned normal or shear strength. Failure of a bond leads to a force redistribution around the breakage that can lead to further breakage. The forces in the bonds can be examined at any time during the simulations. A comparison of bond forces for the thermally homogeneous and heterogeneous specimens demonstrates that the bond forces are evenly distributed in the former, whereas the situation inside the latter is less smooth, and higher forces are concentrating around the particles with higher thermal expansion coefficients (Figure 4-3). Thus, the local force field is at any moment more complex inside the thermally heterogeneous material than it is inside the homogeneous material. This, however, did not significantly affect the macroscopic, large-scale behavior.

In the numerical experiments, AE events were simulated. Figure 4-7 shows the AE events before and after the failure. The pre-failure events are isolated and randomly located, and are typically related to the formation of only one microcrack. Several cracks are clustered to a larger AE event when they occur close together both in space and time. The failure happens so fast that it is recorded as one large AE event, even though the event consists of a multitude of microcracks. The magnitudes of the events in the models range from -5 to -3. The used numerical AE routines are based on the work by Hazzard & Young (2002). In the laboratory experiment, the amount of tensile and shear events was about equal during the pre-failure stage. In the numerical models, the pre-failure events were dominantly tensile (80-85%).
with a few shear events concentrating around the borehole. The source type classifications of the model events (Figure 4-7) were done based on the moment tensor isotropic components (k). The b value calculated from the synthetic AEs of the models varied between 1.0 and 2.0. This value relates the frequency of the seismic events to the event magnitudes. It varies slightly, but is often close to 1.0 (Lockner, 1993). The magnitudes of the events were not available for the laboratory experiment.
Figure 4-7. Above - AE events classified by source type. Below - Pre- and post-failure AE event locations (circles) and moment tensors (vectors). Short red lines show bond breakages. Due to plot scaling, larger magnitude force vectors exceed the plot area. The post-failure plot also includes pre-failure events. Modeling case mC_tF.
4.1.5 Sensitivity of the models

The thermal and mechanical properties of the models were varied to investigate the sensitivity of certain parameters, such as particle size. This was necessary in order to ensure that the models replicated observed trends, and to provide additional confidence in the modeling technique.

The particle size affects the material’s mechanical properties as has been shown in various cases documented by Potyondy & Cundall (2004). Thermal expansion is represented as a relative change of the size of the object due to a temperature increase; therefore the expansion is independent of the size of the object. In accordance, the particle size of a PFC model should not affect the macroscopic thermal expansion of the material. In order to confirm this, the macroscopic thermal expansion coefficients of the different resolution specimens were measured using PFC2D. These numerical samples were square-shaped. The number of particles in the coarse model was about 6000, and the corresponding number in the fine model was about 14000. Three different values of the thermal expansion coefficient were assigned to the different models’ particles; two homogeneous cases and a heterogeneous case (similar to thermal materials presented in Section 4.1.2). A total of six different cases were run; three with coarse models, and three with finer models. The models were subjected to uniform temperature differences of 100 degrees, and the resulting thermal expansion (strains) was measured after the heating phase, as shown in Table 4-4. Thermal expansion of the coarse and fine resolution numerical models was equal when the same microscopic expansion coefficients were used for the model particles. It was therefore verified that particle size does not affect the elastic thermal expansion of the PFC2D material.
Table 4-4. Thermal expansion of coarse and fine PFC2D specimens.

<table>
<thead>
<tr>
<th>Input thermal expansion property set</th>
<th>coarse</th>
<th>fine</th>
</tr>
</thead>
<tbody>
<tr>
<td>A: 3.5x10^-6</td>
<td>0.00035</td>
<td>0.00035</td>
</tr>
<tr>
<td>A: 16.5x10^-6</td>
<td>0.00165</td>
<td>0.00165</td>
</tr>
<tr>
<td>A: 25, 15, 10x10^-6</td>
<td>0.00172</td>
<td>0.00172</td>
</tr>
</tbody>
</table>

One of the key issues in this type of thermal modeling is how to apply heat to the system. In the laboratory experiment, the heater was placed in the central borehole. In the numerical experiment, it was modeled by a layer of particles lying along the borehole wall, which were identified as the heater element. Like the heater in the laboratory experiment, the temperature of these particles was gradually raised to a specified temperature. If the temperature was increased too fast, the heater element broke, and heater particles detached from the specimen due to a thermal shock effect. Several trial runs were needed in order to establish a procedure that provided heating that was smooth enough, while limiting the process to a reasonable modeling time. Although the current heating procedure works well with the model setup, it might have to be modified if the model properties were radically changed.

Another issue with the heater was that a small number of heater particles detached from the borehole wall during the modeling. This was due to the high stresses generated between the heater particles. The detachment usually happened after the main failure, and thus did not have a major effect on the model behavior. In some cases, however, the heater failed before the specimen, which resulted in an unsuccessful experiment. For comparison, a specimen without the central borehole was generated, and the same thermal experiment was conducted...
with this second specimen. The comparison plot of the two modeling cases is shown in Figure 4-8. The results showed that in most cases, the macroscopic fracturing was similar to that described previously. The main difference was that the amount of cracking around the borehole decreased significantly. This is thought to be due to the additional confining pressure provided by the expanding heater particles. In cases where the borehole was present, the heater element was able to move towards the free space, affecting the radial pressure felt near the borehole, and thus failed to provide any supporting confinement. Moreover, the detached particles released the stresses around the borehole, and therefore reduced the support force even further. By filling the hole with particles, a dramatic change in stress conditions near the hole was produced. In the laboratory experiment, there might have been slight confinement due to the fine sand that was added to the borehole (in the area around the heater).

An interesting result of the laboratory experiment was a radially spreading cracking pattern that originated from the borehole. The shorter crack features can be identified from the AE in Figure 4-2 (reproduced in Figure 4-9). A similar observation was made during a hydrofracture experiment, in which fluid pressure applied to a central borehole was used to crack a cylindrical rock specimen (Al-Busaidi, Hazzard & Young, 2005). The reasons for this cracking are not fully understood. One hypothesis is that the configuration minimizes cracking energy, i.e. it is the most stable state under the loading conditions (Jagla & Rojo, 2002). This is based on the assumption that cracking occurs in certain sections around the borehole in such a way that preferred conditions will be met. This could explain why radially spreading cracking was not observed in the numerical models with the central borehole. The cracking started at the outer boundary, propagating inward, and there was not enough
cracking near the borehole to initiate the aforementioned stress re-orientation process. The models that did not have the borehole, however, exhibited minor, radially spreading cracking in three opposite directions (Figure 4-9) similar to that generated in the laboratory experiment of the heated cylinder, as well as in the hydraulic fracturing models. The models without boreholes exhibited different stress states, which affected the damage formation. It is believed that the additional outward pressure of the confined and expanding heater particles constitutes the main difference between the two heated model types. During a hydraulic fracturing experiment (Al-Busaidi, Hazzard & Young, 2005), the fluid is pressurized in the borehole, producing an outward oriented pressure similar to that produced by the thermal experiment without the central borehole.
Figure 4-8. Comparison of microcracking with and without the central borehole, otherwise the specimens (mC_TH) were exactly the same. The filled borehole provides significant confinement to the specimen near the heater, thus preventing cracking around the borehole.
4.1.6 Application of the outcome

In many nuclear waste disposal concepts, the fuel canisters are placed in vertical boreholes drilled in the floors of the disposal tunnels. The spacing of the holes will depend on the mechanical and thermal properties of the host rock. One of the thermal issues is thus the effective distance of the thermal stresses. During the canister placement, a temperature gradient is created between the last disposed canister and the next empty borehole. It is therefore of vital importance to determine whether this thermal gradient is great enough to
produce stress-induced cracking near the empty borehole, and to determine at what distance the effect would be most insignificant. These important questions can be addressed using a thermo-mechanical PFC model.

The 30 cm granite sample used in the laboratory experiment turned out to be too small and exhibited high tensile hoop stresses. It was hoped for that the heating would fracture the sample with cracks propagating from the hole. However the size of the sample with the applied heating scheme generated high tensile stresses at the perimeter of the sample and the sample failed by a fracture which initiated from the outer part of the rock cylinder. An example of the strengths of the PFC modeling approach is to determine a sample size that would not crack around the perimeter when heated. Furthermore, we must ask whether it is still feasible to study the size of the rock sample in the laboratory environment. In response to this question, a 60 cm diameter numerical specimen was generated and subsequently heated. The numerical specimen had the same material properties as the previous model mC_tF. The thermally induced cracking started near the heater, and then propagated in two opposite directions: outward and inward. The results showed that the size of the PFC2D model was large enough to prevent unacceptably high hoop stresses at the specimen perimeter. However, a similarly sized rock sample would weigh about 190 kg, compared to the 40 kg of the 30 cm sample.

4.1.7 Conclusion of the heated cylinder simulations

This concludes the presentation and discussion of the first numerical modeling experiment with PFC2D, which combined thermal loading and AE monitoring. The PFC2D numerical results were directly compared to the corresponding laboratory experiment. The AE data
shows a number of trends observed in the models; initial scattered microcracking, microcracking propagating outwards from the central borehole (the model featuring a filled borehole), and lastly microcracking propagating inwards from the perimeter (as observed in the other models). It can be concluded that the locations of the microcracking observed in the model and in the experiment are qualitatively similar; this is the case, for example, for the modeling case mC_tF. The model successfully captured the behavior of the laboratory experiment, i.e. the macroscopic tensile failure driven by high hoop stresses in the perimeter of the specimen.

Earlier approaches to quantifying thermal damage of brittle rocks have lacked the ability to produce spontaneous cracking behavior. Cracks had either been previously introduced to the material, or they propagated via prescribed paths. In the present study, however, the thermally induced cracking initiated and propagated based on the system state observed at any moment, and produced a propagating failure comparable to the results of the previous laboratory experiment.

The specimens for LdB granite were created using described material genesis procedures (Potyondy & Cundall, 2004). Most of the mechanical properties were kept constant, but the linear thermal expansion coefficient was varied, and hence several numerical specimens with different $\alpha_t$ values were built. The failure temperature was found to depend on the value of $\alpha_t$ as well as on the material strength; stronger material and lower $\alpha_t$ values produced higher failure temperatures. Figure 4-10 shows these relationships schematically. Also, thermally homogeneous and heterogeneous material types were used but thermal material type did not have a significant effect on the failure temperature.
Figure 4-10. Unitless presentation of the relation between the observed failure temperature, the applied thermal expansion coefficients, and material strengths for the PFC2D models. The value of the thermal expansion coefficient increases and the material strength decreases along the horizontal axis. The triangles represent the results from modeling, the line is a trendline.

4.2 Heating of Westerly granite and PFC3D samples

The following section describes steps taken in order to implement and test the enhanced particle clustering routines in PFC2D and PFC3D. The numerical specimens represented the mechanical properties of Westerly granite. The results from the simulations were compared to the pre-existing laboratory data. After the calibration runs, the PFC3D cubic specimens were heated up to 450°C. During the heating, cracking, AE activity and the temperature
evolutions were monitored. P wave velocity measurements were conducted for each of the numerical specimens. The responses were compared to similar thermal laboratory data.

4.2.1 Experimental data

Data from the thermal laboratory experiments by Nasseri, Schubnel & Young (2007) was compared to the numerical results obtained in this study. The researchers slowly heated four sets of Westerly granite samples to 250, 450, 650, and 850°C. Thermal cracking decreased the measured fracture toughness, but also the dynamic elastic properties such as P wave velocities. When heated to 850°C, the maximum velocity decreased by 80%. The biggest drop occurred between 450 and 650°C, and was due to changes in the properties of the quartz mineral. Microscopic study of the used material revealed that the increase in the grain boundary cracking was due to the heating.

4.2.2 Numerical models

The numerical specimens for Westerly granite were created based on the strength and deformation properties recorded by Janach (1977) and Pettitt (1998). The specimens were parallel-bonded, and created using the material genesis procedures described in (Potyondy & Cundall, 2004). In order to determine the specimens’ macroscopic properties, uniaxial and triaxial tests were performed. The specimens were rectangular (PFC2D) and cylindrical (PFC3D), with a height of 120 mm and a width/diameter of 54 mm, and had approximately 4000 and 80000 particles, respectively. The PFC specimens used clusters to represent the mineral entities. The bond strengths inside a cluster (intracluster) were two times the bond strengths between the clusters (intercluster). The strength ratio was rationalized with a study
by Tromans & Meech (2002). A single cluster was composed of about 7 particles. Table 4-5 lists the main PFC2D and PFC3D microparameter values.

The macroscopic deformation and strength properties of the numerical specimens and of the Westerly granite are given in Table 4-5. The strength envelope of the Westerly granite yielded a friction angle of 49° and cohesion values of 43 MPa. For PFC2D and PFC3D specimens, the values were 25° and 73 MPa in confining pressures of up to 100 MPa. Figure 4-11 shows the strength envelope for the PFC2D and PFC3D materials, as well as that of the Westerly granite after Janach (1977). The mismatch of the strength envelopes is a well-known limitation of PFC materials, as recorded by Potyondy & Cundall (2004), and is attributed to the simple shape (disk/sphere) of the modeling element. The use of particle clusters of an average size (featuring seven particles) did not produce any significant improvement for the issue.

For the sake of being able to proceed more straightforwardly, the numerical heating experiments used 45 mm PFC3D cubical samples. The specimen had 48083 particles, with an average particle diameter of 1.3 mm. The specimen had 9661 clusters, divided into three equally sized groups (Figure 4-12). The particles belonging to the each group were assigned different thermal properties that resembled the homogeneous microstructure of the Westerly granite. The thermal expansion coefficients of quartz, microcline (feldspar), and plagioclase were adopted from (Fei, 1995). The applied values were 25, 10, and 5 [x10^{-6} °C^{-1}], respectively. The mineralogical composition of the Westerly granite consists of 27% quartz, 36% microcline, 30% plagioclase, and 7% mica and others. The mean grain size is 0.75 mm. (Nasseri, Schubnel & Young, 2007).
Table 4-5. The key PFC2D and PFC3D material properties.

<table>
<thead>
<tr>
<th>PFC2D input parameter</th>
<th>PFC2D</th>
<th>PFC3D</th>
<th>Westerly granite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Microproperties (input)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Particle density [kg/m³]</td>
<td>3170</td>
<td>3170</td>
<td></td>
</tr>
<tr>
<td>Contact and bond stiffnesses [GPa]</td>
<td>55.0</td>
<td>55.0</td>
<td></td>
</tr>
<tr>
<td>Bond strengths for intra/intercluster [MPa]</td>
<td>295/145.0</td>
<td>320/160</td>
<td></td>
</tr>
<tr>
<td>Bond strength deviation</td>
<td>23%</td>
<td>23%</td>
<td></td>
</tr>
<tr>
<td>Minimum/average particle diameter [m]</td>
<td>0.01/0.013</td>
<td>0.01/0.013</td>
<td>0.00075</td>
</tr>
<tr>
<td>Macroproperties (output)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of particles in UCS/triaxial testing</td>
<td>4000</td>
<td>80000</td>
<td></td>
</tr>
<tr>
<td>Uniaxial compressive strength [MPa]</td>
<td>226</td>
<td>200</td>
<td>229</td>
</tr>
<tr>
<td>Young’s modulus [GPa]</td>
<td>64</td>
<td>57</td>
<td>64</td>
</tr>
<tr>
<td>Friction angle, cohesion</td>
<td>25°, 73 MPa</td>
<td>25°, 73 MPa</td>
<td>49°, 43 MPa</td>
</tr>
</tbody>
</table>

Figure 4-11. Strength envelope of the PFC materials and the Westerly granite, confining pressure of up to 100 MPa.
Figure 4-12. PFC3D cube with a side length of 45 mm, showing the three cluster groups. The size of the clusters varies between 2-5 mm, compared to the Westerly granite’s grain size of 0.75 mm.

4.2.3 Simulation response and comparison with laboratory data

The heating was simulated by directly and uniformly increasing the particles’ temperature in increments of 5°C until the target temperature was reached. After each incremental temperature rise, the model was timestepped to the mechanical equilibrium before the temperature was further increased. Four experiments were conducted, in which specimens were heated up to 150, 250, 350, and 450°C, respectively. The phase transition of the quartz mineral near 600°C changes its thermo-mechanical response (Simmons & Cooper, 1978).
This phenomenon was not incorporated into the thermal routines of the PFC3D, and the numerical simulations’ maximum temperature was therefore capped at 450°C.

Seismic velocities of the numerical specimens were measured by propagating pressure waves through the PFC3D cubes. Ricker waveforms were used for transmitting. The velocity was calculated from the time difference between the first peaks of the source and received waves (Hazzard & Young, 2004). The dominant frequency of the wave was set depending on the particle sizes in the specimen. It varied between 200 kHz and 400 kHz.

Cracking and the interpreted AE events were monitored during the thermal simulations. Seismic velocities of the numerical specimens were measured before and after each heating. Figure 4-13 shows the P wave velocities, AE event count, as well as the percentage of broken bonds with respect to the thermal treatment. The observed behavior corresponds to the laboratory observations. Damage increases with the temperature. The measured P wave velocities decrease with the damage, and there is an increase in AE count.

With temperatures of up to 250°C, the normalized P wave velocity trend is strikingly similar to that of the laboratory experiment. Once temperatures go above 300°C, the velocity measurements ceased to be successful due to the noise in the damaged specimens. The velocity routine monitors the movement of the receiver particle, while the noise represents random particle movement. In the numerical modeling method, a particle velocity is never zero (unless fixed in space), and during the heating the movement increases as the damage is increasing, disguising the actual arrival of the propagated wavefront in the recorded waveforms. At a temperature of about 400°C, the PFC3D specimen starts to disintegrate, and no velocity measurements could be carried out due to the extensive damage. At this point,
more than 30% of the particle bonds are broken. In the laboratory experiment, the rock is still intact at temperatures of 850°C.

The observations of the cracking in the PFC3D specimens show that cluster boundary cracking is dominant (Figure 4-14), and thus similar to the grain boundary cracking in the laboratory experiment. The strong thermal expansion contrasts between the adjacent particle clusters give rise to high stresses. The numerical specimens are structurally perfect in the sense that there are no microcracks or flaws present. When a specimen is heated, at some point there is no more space for clusters to expand, and local cracking subsequently leads to a major material failure and to the specimen’s fragmentation. Another hypothesized reason for the extensive failure is the coarse particle size in relation to the specimen size. The particular particle size was chosen so that the simulation time would still be manageable. If the particle size would be halved, the simulation time for each model run would have increased from days to weeks.
Figure 4-13. Evolution of the normalized P wave velocity PFC3D (circle) and laboratory data (triangle), PFC3D AE count, and normalized number of broken bonds (square) in relation to the rising temperature.
Figure 4-14. Microcracks formed mainly between the particle clusters in the PFC3D simulation of the heated Westerly granite cubes.

4.2.4 Sensitivity of the wave velocity measurements in PFC2D

The sensitivity study was conducted in order to understand the effect of the input parameters in the P wave velocity measurement results. In the study, P waves were propagated 100 times
through a PFC2D specimen, each time with different frequencies and amplitude values. The width and height of the numerical specimen were 54 mm and 120 mm, respectively. The average particle diameter was 1.3 mm, and there were about 4100 particles. The measured unconfined compression strength of the specimen was 225 MPa. The values for Young’s modulus and Poisson’s ratio were 64 GPa and 0.25, respectively. The input frequency value was varied between 180 kHz and 360 kHz, and the amplitude value between -0.01 and -10.0. Negative value means that the first movement of the input wave was towards the negative axis direction (towards the center of the specimen). The mean measured P wave velocity value was 5360 m/s. The standard deviation in the 100 experiments was 330 m/s, with the largest and the smallest values being 5700 and 4300 m/s, respectively. The results are collected in Figure 4-15, and are shown in a line graph form in Figure 4-16.

The study concludes that the choice of the input parameter values as well as of frequency and magnitude notably affects the measurement results. The measured velocity increases with the increased input frequency value. For a changing input magnitude value, there was observed a magnitude range within which the measured velocity value stayed constant; once the input magnitude value drifted from that range, however, the velocity values deviated rapidly. It was also clear that the two parameters were dependent. Simultaneous increase of both values seemed to keep the measured velocity value near constant. Furthermore, it was found that the frequency value is dependent on the particle size, as described earlier. The study emphasizes the sensitivity of the measured values with regard to the input parameters. This is especially important when comparing the velocity values of different simulations, or when comparing simulations with real experiments. One should keep the chosen frequency and amplitude values constant when conducting velocity studies in a single PFC material.
Figure 4-15 Results of 100 wave velocity measurements from a PFC2D specimen. The velocities are shown in relation to the input frequency and amplitude values. Color gradient emphasizes the differences in the velocity values. The most frequently occurring value (mode) is 5580 m/s.
Figure 4-16. P wave velocities with respect to input wave frequency (value axis) and amplitude (series) values. The numerical data is presented in the previous figure.

4.2.5 Conclusion of the heated cube experiment

Particle cluster groups were introduced into PFC3D material in order to better model the thermal behavior of hard rock. The clustered specimens were calibrated to match the mechanical properties of Westerly granite. The comparison of the mechanical data was done using standard uniaxial and triaxial compression tests with confining pressure of up to 100 MPa. Cubic PFC3D specimens, each having about 10000 breakable particle clusters, were heated up to a temperature of 450°C. Heating induced damage was observed by AE monitoring and P wave velocity measurements. The comparison of velocity measurements against the existing laboratory data showed similar behavior up to 250°C.
4.3 Summary of the laboratory scale modeling

The first laboratory scale modeling case dealt with a heated cylinder sample of Lac du Bonnet granite, and was described in Section 4.1. The circle presentation of the cylinder was generated with the PFC2D software. The specimen’s core was heated, and the synthetic AEs were recorded during the heating. The sample ultimately failed due to the high tensile hoop stresses that caused fracture propagation from the sample’s outside towards the inner parts of the sample. The temperature difference between the core and the outer surface caused the tensile stresses to build up at the outer perimeter. This was also analytically shown by Equation 3-5, presented in Section 3.2. During the subsequent simulations, additional observations were made: Increasing the thermal expansion coefficient has proved to reduce the failure temperature in the cylinder, while an increase in the material strength raised the failure temperature. When the material strength was decreased, the observed failure type changed, from a fracture plane propagating from the perimeter of the sample toward the centre to extensive cracking around the borehole (‘borehole crushing’) without any propagating fracture planes. When comparing modeling cases featuring specimens constructed with different particle groups (each having different thermal expansion coefficients) to the isotropic case in which only a single coefficient value was assigned to all the particles, it was observed that the actual failure temperature remains roughly the same, but that the amount of the initial microcracking was less in the isotropic case.

The second laboratory scale modeling case simulated Westerly granite cubes, using PFC3D software, and was described in Section 4.2. The 45 mm cubes were uniformly heated to a temperature of 450°C. The specimens were constructed using particle clusters. Three
different thermal expansion coefficient values were assigned to the different particle clusters. The particle bond strengths between the clusters were half of the bond strengths between the particles inside a cluster. This constellation was chosen in order to imitate the properties of the granite forming minerals, quartz, microcline, and plagioclase. The P wave velocity measurements were conducted after each completion of a 100°C heating increment, and were compared to the available laboratory data. The trend of the velocity change from the initial untreated conditions was found to correspond to the experimental data of temperatures of up to 250°C. After further heating, the PFC3D specimens became so damaged that the velocity measurements could not be used. At 250°C, about 8% of the bonds in the PFC3D specimen were broken, and further heating caused increasing damage. At 350°C, nearly 25% of the bonds were gone; at 450°C, nearly 30%. In PFC, a seismic wave propagates in particle contacts and bonds. Therefore, the more deleted bonds and probable gaps there are, the harder it is for the wave to advance. The wave energy then scatters, and does not reach the receiver. If a stronger (higher amplitude) wave is input, it might reach the receiver, yet it is more likely that the strong particle movements would cause further, unrealistic damage to the PFC specimen. The other dissimilarity between real granite and the PFC3D cubes is the near perfect undamaged and tight packing of the PFC particles, as compared to the ever-present microcracking in real rock. The lack of existing microcracks in PFC a material would produce slightly exaggerated damage during the heating phases, since there is no space for the particles to freely expand without immediately affecting the neighboring particles.

One of the limitations in the PFC2D and PFC3D models was the fact that during the cyclic heating, no cracking occurred in the cooling phase. The cracking would increase only once the temperature had exceeded the maximum temperature value of the previous heating cycle.
By introducing more complex particle cluster shapes, it was hypothesized that these would allow stresses to be locked during the thermal cycling that then could lead to additional cracking when the specimen is cooled. Another phenomenon observed during the laboratory heated cylinder experiment was the seismic activity (AE events) along the formed fracture plane, occurring when the sides sheared against each other. This was not observed during the PFC2D simulations. By definition, microcracks form in PFC models due to the bond breakages. Therefore, shearing of already-cracked surfaces does not produce any observed events. Furthermore, the stress conditions in the heated core affected the macroscopic failure behavior. To summarize, filling the borehole with particles changed the damage pattern from displaying an inward-propagating failure front to microcracks spreading from the borehole in a star-like shape. The details are discussed in Section 4.1.5.

The synthetic acoustic events were recorded during the PFC2D modeling of the heated cylinder experiment. The results are described in Section 4.1. Qualitative comparison with the laboratory data showed similar responses during the experiment. In the beginning, there were only few events throughout the sample. In later stages, they were concentrated to the large propagating fracture. In comparison to the magnitudes recorded during the major failure, the early event magnitudes were small. However, quantitative comparison was limited because of the differences between two-dimensional synthetic seismicity and the full three-dimensional acoustic emission events of the real world. The moment tensors, used to construct various seismic parameters such as T-k plots, cannot be generated from the 2D data. Thus, the comparison presented in Section 4.1.4. only used the moment tensor isotropic components. The observed synthetic seismicity was also found to be dependent on the shear wave velocity value. Velocity values are input parameters, and are used to cluster individual
microcracks to larger AE events in the numerical routine. Different shear wave velocity values thus produce slightly different AE events in the model. This was tested by running the same model with varying velocity values, and by observing the resulting differences in the AE event counts and magnitudes. It was found that the range of the event magnitudes does not change much, but that higher input velocity value produces higher amounts of the AE events. Velocity values were varied between 1500 and 4500 m/s. The measured event magnitudes varied between -5.2 to -3.0, and the total number of AE events ranged from 171 to 188. In the simulations, presented in Section 4.1, the shear wave velocity value was set to 3000 m/s, which was about the value of the LdB granite.

During the wave propagation experiments documented in Sections 4.2.3 and 4.2.4, it was observed that the measured P wave velocity is highly dependent on the specific input frequency and amplitude values, and is furthermore related to the particle size. In the conducted sensitivity study, the P wave values were propagated 100 times through the PFC2D specimen, with different frequency and amplitude values. Input frequency and amplitude values were varied in a 100% range. The measured P wave velocity value was found to vary in a range of about 30%. It was concluded that the choice of the input parameter values notably affects the measurement results. To summarize, it can be stated that the measured velocity increases with the input frequency. The effect of the input magnitude is less notable, but the two parameters are co-dependent. This finding is important for velocity comparison studies that either concern different PFC simulations or a PFC simulation paired with a real experiment.
5 FIELD SCALE MODELING

5.1 Underground thermal experiments

Disposal in underground cavities is an extensively studied method for the management of used nuclear fuel. One of the studied aspects has been the thermal effect on the surrounding rock material. Between 1993 and 1996, Atomic Energy of Canada Limited (AECL) conducted a heated failure test (HFT) (Read et al, 1997). The test investigated the effects of thermal loading on the excavation damage development. In the test, boreholes were drilled on the floor of the Mine-by tunnel. During the four stages of the test, a total of five 0.6 meter diameter holes were drilled. The rock surrounding the holes was heated with heaters located about 1 meter from the hole walls. AE monitoring provided a means of identifying the damage development in the test area. Numerical modeling was used to interpret the borehole breakouts, which were mainly due to increased tangential stresses.

In 2003 and 2004, a similar experiment was conducted by Swedish Nuclear Fuel and Waste Management (SKB). The Äspö pillar stability experiment (APSE) studied the progressive failure in a highly stressed pillar (Andersson, 2007). In the experiment, an experimental tunnel was excavated perpendicular to the maximum principal stress the rock was exposed to. Additionally, the tunnel cross-section was shaped in such a way that the stress effect below the tunnel floor was maximized. Two 1.8-meter diameter boreholes were drilled to the floor in a distance of 1 meter from each other so that a pillar was created in between (Figure 5-1). Pre-experiment studies predicted significant stress magnitudes in the pillar (Andersson et al, 2003). The other borehole was pressurized, so that the borehole walls were confined. The rock surrounding the holes was heated with four heaters, which created thermal stresses.
in the pillar area. The experiment was monitored with an AE system (Haycox, Pettitt & Young, 2005). Borehole breakouts developed close to the pillar’s center, where the tangential stresses were highest. The effect of the confining pressure was evident, as AE events were recorded in the unconfined hole, but remained less noticeable in the other, confined borehole (Figure 5-2).

Between 1997 and 2004, a tunnel sealing experiment (TSX) was conducted in the same underground facility as the earlier mine-by heated failure test. In the experiment, a tunnel with an elliptical cross-section was excavated parallel to the maximum principal stress direction. The tunnel was filled with sand and sealed with bulkheads at both ends. The tunnel was then pressurized to 4 MPa, and heated by injecting 85°C water in the center of the chamber (Figure 5-3). The rock mass response was monitored with an AE/MS instrumentation method (Haycox, Collins & Pettitt, 2004). Major portions of the seismic events were located in the roof region, migrating over time from the center outwards towards the tunnel’s ends. The lesser amount of seismic events recorded at the tunnel floor was thought to be due to the confinement provided by the sand and the water in the floor region.
Figure 5-1. APSE experimental geometry and the modeled maximum stresses after the excavation stage; magnified view of the pillar area at right. (after (Andersson, 2007)).
Figure 5-2. APSE experiment, AE events during the heating stage shows a clustering of events along the length of the holes. (after Haycox, Pettitt & Young, 2005).
Figure 5-3. TSX experiment, 13-meter tunnel is sealed at both ends, filled with sand, and heated by injecting hot water to the chamber. (after (Guo et al, 2005)).

5.2 Discussion on PFC modeling possibilities

Each of the in-situ experiments could be modeled with the PFC method, given that necessary computational resources are at hand. Each of the cases has interesting features that could be studied further with the help of numerical simulations. In the heated failure test, the experimental tunnel had notches on the floor and roof that were developed during the excavation. The notch development without thermal effects had previously been modeled with the coupled FLAC-PFC2D method (Figure 5-4), for example by Hazzard & Young.
During the heated failure test, the notch at the floor activated what was observed as increasing AE events in that region.

During the SKB Pillar stability experiment, increasing AE activity was observed, as expected, in the highly stressed pillar area. In addition, AE events were clustered along a pre-existing fracture zone, which penetrated the pillar horizontally. This was observed during the heating phase, and can be seen in Figure 5-2. This observation could be an interesting challenge for a PFC modeling study. In the TSX, the sand filling procedure applied a pressure to the tunnel floor, where MS monitoring subsequently recorded less damage than in the roof region. It was also noted that the event magnitudes were smaller during the heating, when compared to the excavation phases.

If considering modeling the APSE case, the model should take into account the whole experimental region including the tunnel. The complex experimental geometry significantly affects, as expected, the stresses at the pillar area. Additionally, the PFC model particles should be small enough to capture the significant cracking in the pillar region. The requirements render the case computationally unrealistic for modeling, unless the simulation could be parallelized using several computer processors. However, the current PFC3D version (3.00) does not support parallel simulations for thermal problems. Similarly, the mine-by heated failure test has a tunnel geometry that affected the stress state at the tunnel floor where the experimental holes were located. In this design, the interesting notch feature at the tunnel floor is furthermore suspended in a stable-unstable state, where slight changes in the boundary conditions affect its development. In order to simulate this realistically, the notch should be left to generate itself during the tunnel excavation phase. Therefore, a full
tunnel scale model is required. Also, since the important part in the notching process is the stress conditions that are acting at its apex, there should be enough model particles at that region. These prerequisites make the case difficult to model on a single computer running PFC2D or PFC3D.

Compared to the other cases, the TSX has a less complex geometry. A full-scale PFC3D model would involve significant computational requirements. It is possible, however, to approach the case with a PFC2D model. Such a model would display some similarities to the heated cylinder experiment described in Section 4.1. The main differences are that the TSX chamber has sand filling, which provides confinement on the floor by gravitational effects, and that there would be in-situ stresses.

Figure 5-4. Notch development at the mine-by tunnel; Recorded (left) and PFC2D simulated (right) AE events at the tunnel roof during excavation (after Hazzard & Young, 2004).
5.3 Tunnel sealing experiment (TSX)

The main objective of the TSX was to study issues related to the full-scale bulkhead seals of underground repositories for radioactive waste. The experiment included two tunnel bulkheads; one composed of clay blocks, and the other constructed using concrete. The tunnel was 13 meters long, 4.375 meters across, and 3.75 meters high, with an elliptical cross-section. In order to minimize the effects of the stress concentrations around the tunnel perimeter, it was oriented parallel to maximum stress exposure. The experiment consisted of the following phases.

- Excavation of the tunnel by the drill and blast method.
- Drilling and rock cutting of the seal regions.
- Building of the clay seal.
- Filling the chamber with sand.
- Building of the concrete seal.
- Pressurizing of the chamber.
- Heating of the chamber by injecting hot water in the chamber’s center.
- Cooling and depressurization of the chamber.

Over the period of 7 years, the experiment was monitored with AE/MS systems, covering all of the experimental phases (Haycox, Collins & Pettitt, 2004). Seismic activity around the tunnel indicated that time-dependent microcracking occurred for years following the excavation. Heated water was injected through boreholes to the center of the chamber. The amount of confinement by sand filling arrested the cracking process, but the heating caused the cracking to start again. The hottest region was in the center. Seismic activity was initially
located at the roof above the heated region, but over time the events migrated from the center towards the seals, as the heat spread slowly in the filling material and rock. A clear relationship was observed between the increase of the temperature and the increase in the microseismic events, Figure 5-5.

Figure 5-5. Summary graph showing the cumulative number of events above and below the TSX tunnel, along with the pressure inside the chamber and the temperature in a borehole adjacent to the chamber during the experimental phases of the TSX. (from Haycox, Collins & Pettitt, 2004).
Seismic activity was highest during the excavation phases, and 95% of the events occurred within 1.4 meters from the chamber walls. During the heating phase, the events did not exceed beyond the initial excavation perturbation zone. It was interpreted that there was an increase in crack densities in the areas of previous damage. The MS observations clearly indicated that during the heating phase, there was less activity in the floor region than in the roof, as shown in Figure 5-6. This was thought to be due to the confinement provided by the sand filling.

Figure 5-6. Microseismic events of the Tunnel Sealing Experiment during the heating of the chamber from 25 September 2002 to 17 September 2003. Top and side views show the events clustering mainly to the roof region. (after (Haycox, Collins & Pettitt, 2004)).
During the heating phase, seismic velocities were measured around the clay bulkhead, as documented by (Collins et al, 2003). Changes in measured velocities can be attributed, for example, to increasing microcracking, changes in a stress state, and the reaching of a level of saturation. Increasing microcracking would lead to reduced velocities. Increased fluid saturation of cracks and stress increase would lead to a P wave velocity increase, depending on the stress orientation in relation to the crack orientation. During the heating period, the velocities were measured once a day. Raypaths were concentrated around the clay bulkhead, with some raypaths also covering regions along the sidewall and below the TSX chamber. Most cracking occurred in the roof region, but unfortunately, no velocity data was recorded from that part of the rock mass. The results showed an increase in velocities during the heating. The greatest increase took place at the sidewalls. It was suggested that the thermal stresses were closing the existing microcracks in the walls, as compared to the floor region, where the cracks were mostly closed prior to the heating, by the pressure from the filling material.

Figure 5-7 shows the raypaths, coded P3-R4 and P3-R16, and the calculated velocity changes (the former going through the floor area and the latter through the side wall). The velocity passing through the floor showed an increase of +20 m/s during the heating period, compared to an increase of +40 m/s in the sidewall. It was hypothesized that those velocity measurements were not affected by the microcracking in the chamber walls.
Figure 5-7. P and S seismic wave velocity changes for raypaths P3-R4 (below floor) and P3-R16 (side wall). (after (Collins et al, 2003)).
The TSX tunnel was oriented parallel to the maximum principal stress direction. The intermediate stress was oriented horizontally, and the minimum stress sub-vertically. The average magnitudes of the stresses were 60, 45, and 11 MPa. In the two-dimensional PFC2D analysis, the stress magnitudes 45 and 11 MPa were applied. The ratio of the stresses is about 4. Based on the well-known Kirsch solutions for a stress state around a perfectly circular opening (for example (Brady, 2004)), the acting stresses would produce a compression of 120 MPa at the roof and floor. The sidewalls would be in a tensile stress regime of about 10 MPa. Based on the analytical calculation examples in (Hoek, 1980), the stress state was approximated also for the more realistic elliptical shape. As expected, these calculations showed that the tunnel geometry reduces the induced stresses around the opening (Young et al, 2001). At the roof and the floor regions, the maximum stress is acting with a value of about 80 MPa. The wall stress amounts to a value of 10 MPa. Based purely on the stress analysis, one would not expect any significant damage around the elliptical TSX chamber, as there are no tensile stress regions, and the maximum compressive stress value does not considerably exceed the crack initiation stress level of the LdB granite (Read et al, 1997). MS monitoring showed that part of the seismic activity occurred not immediately after the excavation, but in the years following it. This was explained as a corrosion mechanism, in which the rock strength reduces over time, via hydro-chemical processes or under a constant load (this process is also called stress corrosion).
5.4 Modeling approach

The TSX was modeled using the PFC2D software. The modeling approach was similar to the heated cylinder experiment described in Section 4.1. Among the noted similarities was the circular/elliptical opening in the middle of the numerical specimen, as well as the fact that the heating was provided from the opening. The main differences between the two modeling cases were the size of the specimen’s physical dimensions, and the fact that the TSX simulation featured stress boundary conditions. In the cylinder experiment, the sides of the PFC2D specimens were free from any constraints.

Compared to the previous PFC modeling studies, the other significant difference was that in the TSX simulations, gravitational forces were engaged. Furthermore, both parallel-bonded and unbonded particles were present in the TSX models. The unbonded particles were located in the chamber opening, and simulated the filling material. The free particles settled under the gravity, and provided confinement on the floor region. Furthermore, two different heating approaches were considered; one case where the particles inside the opening were heated, and a second case where the particles at the whole perimeter were heated.

In PFC modeling, servo-controlled walls can be used to apply constant stress at the model boundaries. This approach is relatively easy to initiate, and throughout the simulations, the wall stresses are automatically kept constant. The approach can therefore be applied as a constant stress boundary condition. However, due to the particular nature of the PFC modeling method, the stress state inside a model might vary slightly locally and not be exactly the same as the one applied to the walls. This is a significant diversion from a continuum-based modeling approach. The numerical servo-controlled mechanism was used
to apply the stress state to the PFC2D specimens. It maintained the wall stresses at the desired values by controlling the wall velocities, and thus the forces acting to the boundary particles. The approach is described in (Itasca Consulting Group, Inc, 2004a). Two different wall control situations were tested. One case in which the servo-control was acting for the duration of the simulation, and a second case where at the start of the heating period, servo-control of the walls was disengaged and the wall positions were fixed.

The excavation was performed by removing the parallel bonds from the particles located in the chamber area. The particles themselves remained in their locations, and settled to the chamber floor once gravity began to exert its force. The filling material was thus simulated by loose PFC2D particles inside the central opening. During the PFC2D specimen generation, particle packing was optimized by minimizing the space between the particles, and by ensuring that all particles were in contact with neighboring ones. To properly simulate the filling material, the size of the filling particles was thus reduced by 0.5%. The particles settled under the force of gravity, and a small gap was formed between the filling and the chamber roof.

The main interest in the modeling of the tunnel sealing experiment was the heating phase. Of all the TSX in-situ experimental phases, the following were included in the modeling sequences: excavation of the opening, filling of the chamber, and heating of the chamber. In order to simplify the simulations, pressurization of the chamber by fluid was omitted in the modeling sequences. Pressurized fluids are not directly supported by the PFC2D modeling method, and extensive additional development and testing would have been required in order to include this procedure. The two-dimensional PFC2D model was a representation of a
section from the middle of the TSX tunnel. Table 5-1 shows a summary of different modeling cases. These cases also represent the model development history. The first presented TSX simulation case was named Case B. The earlier modeling runs were cases generated during the development and testing of the TSX simulation steps, and are not presented here. For LdB granite, the ratio of uniaxial compressive strength to Brazilian tensile strength is about 20. For a given PFC material, the ratio is always about 5, which represents one of the known issues of the simulation of rock with the PFC method (Section 3.1), and furthermore means that at this time, a PFC material can correctly simulate the strength of either UCS or Brazilian but not both at the same time.
Table 5-1. PFC2D modeling cases of the Tunnel Sealing Experiment.

<table>
<thead>
<tr>
<th>Modeling Case</th>
<th>Model property</th>
<th>Filling material size (with respect to original particle size)</th>
<th>Material strength [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>Off Center</td>
<td>0.995</td>
<td>50/10</td>
</tr>
<tr>
<td>C</td>
<td>On Center</td>
<td>0.995</td>
<td>50/10</td>
</tr>
<tr>
<td>D</td>
<td>Off Center</td>
<td>1.0</td>
<td>50/10</td>
</tr>
<tr>
<td>E</td>
<td>Off Center</td>
<td>0.995</td>
<td>100/20</td>
</tr>
<tr>
<td>F</td>
<td>Off Perimeter</td>
<td>0.995</td>
<td>50/10</td>
</tr>
<tr>
<td>F2</td>
<td>Off Per + center</td>
<td>0.995</td>
<td>50/10</td>
</tr>
<tr>
<td>G</td>
<td>Off Perimeter</td>
<td>0.995</td>
<td>100/20</td>
</tr>
<tr>
<td>G2</td>
<td>Off Per + center</td>
<td>0.995</td>
<td>100/20</td>
</tr>
<tr>
<td>H</td>
<td>Off Per + center</td>
<td>0.995</td>
<td>75/16</td>
</tr>
<tr>
<td>J</td>
<td>On Per + center</td>
<td>0.995</td>
<td>75/16</td>
</tr>
<tr>
<td>K</td>
<td>On Per + center</td>
<td>0.995</td>
<td>50/10</td>
</tr>
</tbody>
</table>
5.5 Numerical models

PFC2D specimens were created based on the material genesis procedure by Potyondy & Cundall (2004). The specimens were of a rectangular shape, with a width of 28 meters and a height of 21 meters. Four surrounding walls bounded the specimen. In the specimen labeled ‘coarse,’ the average particle diameter was 180 mm. The other specimen, labeled ‘fine,’ had an average particle diameter of 90 mm. The number of PFC2D particles in the specimens was 19000 and 76000 for the ‘coarse’ and ‘fine,’ respectively. The thermal modeling stage simulated 12 weeks of heating. This duration was chosen in order to optimize computation time. In the in-situ experiment, the actual heating stage lasted one year. The computational runtime per modeling case was about 30 hours for the coarse models (using a PC with a processing speed of a 3.0 GHz). Figure 5-8 shows the coarse PFC2D specimen with the four bounding walls.

The material properties for the PFC2D models were based on Read et al. (1997) and Martin (1993). The main rock type in the TSX tunnel, located in the Canadian URL, was granite with a grain size of about 5–8 mm. The in-situ strength of the rock was approximated to be about 70-80% of the unconfined compression strength (UCS). In some cases, the in-situ strength was approximated to be as low as 50% of the UCS. The crack initiation stress level is described as $\sigma_1-\sigma_3=70 \text{ MPa}$. The PFC2D material strength (UCS) of the cases H and J is about 75 MPa, which is close to the LdB granite crack initiation stress value. The values for Young’s modulus and Poisson’s ratio are 65 GPa and 0.25, respectively. The density of the rock is 2650 kg/m$^3$. The thermal conductivity $k$ is 3.5 W/m°C, and the specific heat $c$ is 1015 J/kg°C. The background temperature of the rock mass was 14°C. As noted in Section 4.1.2,
the linear thermal expansion coefficient of LdB granite, $\alpha$, varies to some extent. Based on the laboratory scale thermal simulations (Chapter 4, Laboratory scale modeling) a uniform value of \(10.0 \times 10^{-6} \, ^{\circ}\text{C}^{-1}\) was chosen for the TSX modeling, in order to reduce possible combinations of the different modeling cases. The PFC2D material properties are listed in Table 5-2.

During the calibration process, the PFC2D material’s unconfined compression strength as well as tensile strength, via a Brazilian test, were determined. Two differently sized test specimens were created; one was a laboratory scale specimen, the other a large-scale specimen. In both cases, the width-to-height ratios were the same. The height of the laboratory scale specimen was 200 mm, and its width 100 mm. The large-scale specimen was 20 m high and 10 m wide. The tests were performed according to Potyondy & Cundall (2004), and the test results are summarized in Table 5-3. In addition to using the base material strength in the simulations, two further strength scenarios were implemented; these were cases in which the material strength was one and a half times and two times that of the base material strength, respectively. These two cases yielded Brazilian tensile strength values of about 16 and 20 MPa, and UCS values of about 75 and 100 MPa, respectively.

**Table 5-2. The key PFC2D material properties after calibration runs.**

<table>
<thead>
<tr>
<th>PFC2D input parameter</th>
<th>coarse</th>
<th>fine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle density [kg/m3]</td>
<td>3170</td>
<td>3170</td>
</tr>
<tr>
<td>Contact and bond stiffnesses [GPa]</td>
<td>62.0</td>
<td>55.0</td>
</tr>
<tr>
<td>Bond normal and shear strengths [MPa]</td>
<td>35.0</td>
<td>40</td>
</tr>
<tr>
<td>Strength deviation [MPa]</td>
<td>7.0</td>
<td>7.0</td>
</tr>
<tr>
<td>Minimum/average particle diameter [m]</td>
<td>0.14/0.18</td>
<td>0.07/0.09</td>
</tr>
</tbody>
</table>
Table 5-3. UCS and Brazilian tensile strength test results for the PFC2D materials.

<table>
<thead>
<tr>
<th>Specimen size label</th>
<th>coarse</th>
<th>coarse</th>
<th>fine</th>
<th>LdB granite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width, height [m]</td>
<td>0.2x0.1</td>
<td>20x10</td>
<td>20x10</td>
<td></td>
</tr>
<tr>
<td>Mean grain radius [mm]</td>
<td>1.0</td>
<td>100</td>
<td>46</td>
<td>1.5</td>
</tr>
<tr>
<td>Compressive uniaxial strength [MPa]</td>
<td>49.5</td>
<td>48.3</td>
<td>57.6</td>
<td>200</td>
</tr>
<tr>
<td>Young’s modulus [GPa]</td>
<td>73.3</td>
<td>69.8</td>
<td>65.3</td>
<td>69</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.251</td>
<td>0.252</td>
<td>0.238</td>
<td>0.25</td>
</tr>
<tr>
<td>Tensile strength from Brazilian test [MPa]</td>
<td>10.7</td>
<td>9.8</td>
<td>8.9</td>
<td>9.3</td>
</tr>
</tbody>
</table>

Figure 5-8. The model geometry for the TSX simulation. The specimen is parallel-bonded except for the chamber area, which is filled with unbonded particles. Four walls bound the specimen with a width of 28m and a height of 21m.
5.6 Simulation response

After the specimen generation procedures, the TSX model was subjected to a stress installation routine that shifted the sidewalls in order to achieve the desired stress-state in the model. After this, the parallel bonds in the elliptical chamber area (width 4.4 meters, height 3.76 meters) were deleted, gravity was engaged, and the filling particle radii were reduced. The variations of these steps are listed in Table 5-1. The system was then cycled to equilibrium, a process during which any microcracking was recorded. The state of equilibrium represented the TSX chamber after the excavation and filling stages.

Heating was simulated by raising the temperature of the particles in the chamber to a target value of 85°C. Since the filling material had settled under the force of gravity, and created a small gap between the roof and the filling, the roof region was initially not directly heated, because the heat could only conduct between those particles that were in direct contact. Therefore, another heating mechanism, in which the chamber perimeter particles were regarded as part of the heating range, was considered. This mechanism was employed in the modeling cases F and later. The temperature of the particles at the outer boundary of the specimen was fixed to an ambient value of 10°C. The following coupled thermo-mechanical calculation was performed to simulate the heating time of 12 weeks (7257600 seconds), a period during which many parameters, such as temperature, stress values, and formed microcracks, were recorded.

Figure 5-9 shows the temperature histories and the amount of microcracking during the simulation of Case B. The damage that occurred during the excavation and heating stages, as well as the location of the temperature measurements are shown in Figure 5-10. The modeled
responses (especially of the resulting damage) varied to some extent between the different simulation cases. The following two sections present the results from select simulation cases. The subsequent section compares the simulated results to the data of the actual TSX in-situ experiment.

Figure 5-9. Solid lines show the temperature evolution at the sidewall (higher temperature) and roof (lower temperature) during the 12 weeks of heating. The dashed line shows the amount of microcracking in the model. Simulation Case B. The locations of the temperature measurements are shown in the following figure.
Figure 5-10. Microcracking around the PFC2D TSX chamber after the excavation and heating phases shows the difference between the roof and floor area damage. Triangles show the locations of the temperature measurements.

5.6.1 Damage development

In the TSX simulations, the heating and the potential effect of the filling material on the damage development in the floor region were the main concerns. The filling material was simulated by unbonded particles under gravitational loading. The weight of the free particles provided a confinement of about 100 kPa on the floor region, which was about the same as the values recorded in-situ.

Case B was the first successful simulation. The model showed damage around the opening, which after the excavation stage was concentrated at the roof and floor. Figure 5-11 shows
the microcracking occurring during the heating phase, categorized with regard to its location (floor/roof) and type (tensile/shear). Figure 5-12 shows the excavation and the heating-induced microcracks around the TSX opening. As the simulation continued, the effect of the filling material became evident, as it became clear that the cracking in the roof area during the heating phase was predominant, when compared to that in the floor area. At some point during the heating, the damage increased suddenly. During the heating phase, most of the formed microcracks were tensile. The damage extended about 1–2 meters from the tunnel perimeter outwards. In the roof area, the microcracking formed a notch-like shape. The apex of the notch reached about 1.5 meters from the tunnel wall. Surprisingly, the first simple model already captured some of these features, which were hypothetically expected based on the stress orientation and the confinement by the filling material.

During the heating phase, the wall positions were fixed (Case B; wall servo off). As the temperature was raised, the particles expanded, producing increasing forces in the bonds between the particles. The fixed (non-servo) walls confined the specimen and prevented them from expanding at the boundaries. This produced wall stresses that were slightly different from those that had initially been applied during the stress installation procedure. The horizontal stress at the left and right boundary walls was about 41 MPa at the end of the simulation round; the corresponding vertical stress values at the top and bottom walls were 12 MPa. Initial installed stresses were 45 and 11 MPa, respectively.

Case C was similar to Case B, with the difference that the wall servo was continuously engaged. The wall stresses, therefore, stayed at their initial value throughout the simulation. Figure 5-13 and 5-14 show the microcracking during the heating phase and the damage
around the tunnel opening, respectively. The results are very similar, but not exactly the same. The differences are due mainly to the servo-controlled walls maintaining the stress boundary conditions. Another reason for the slight variation of the observed microcracking is thought to be the coarse resolution (i.e. relatively large particles) of the models. Because of the force redistribution that occurs in the model after each breakage, the first microcracks will dictate the subsequent behavior. Random particle packing furthermore provides a natural heterogeneity in the models; no two models are exactly the same. Even with the slight differences between the cases, the large-scale damage formation is similar, and is represented by a notch-like shape in the roof, as well as suppressed damage at the floor.

For two different reasons, the subsequent cases D and E produced hardly any damage at all. Case D was similar to Case B, except that the filling particle radii were not reduced during the simulation. Initial particle packing was rather tight, and because of the radii expansion of the filling material, which was induced by the temperature change, expansion occurred symmetrically, thus providing symmetrical confinement against the chamber walls. The amount of confinement seemed to be high enough to suppress any possible damage. In Case E, the PFC2D material was twice as strong as the material in the aforementioned cases. Otherwise, this case was, again, similar to Case B. Towards the end of the heating phase, only three microcracks had formed in the stronger material.
Figure 5-11. Microcracking and temperature evolution during the heating phase, Case B.
Figure 5-12. Microcracking around the TSX chamber due to the excavation (closed circles) and heating (open circles). Simulation Case B.
Figure 5-13. Microcracking and temperature evolution during the heating phase, Case C.
Figure 5-14. Microcracking around the TSX chamber due to the excavation (closed circles) and heating (open circles). Simulation Case C.

For Cases F and onwards, a different heating mechanism was employed. This mechanism was developed in reaction to the creation of the small gap between the chamber’s roof and filling (as mentioned previously), which prevented the direct heating of the roof region. Initially, the new heating mechanism was designed to affect only the tunnel perimeter particles. After running two simulation cases, however, the new heating scheme also included simultaneous heating of both the filling and the perimeter particles. Cases F and G employed the initially developed new heating mechanism. The cases were later rerun with the final scheme, and were then labeled cases F2 and G2.
Except for the new heating mechanism, Case F2 was again similar to Case B. The simulation also yielded different data than the previous cases. In this case, the damage is more extensive, and appears in a roughly symmetrical fashion after the excavation. Figures 5-15 and 5-16 show the microcracking and temperature evolution of Case F2. During the heating phase, the damage is concentrated in the roof region, although there also is activity below the floor. The material in Case G2 was twice as strong as that in Case F2; except for the heating scheme, it is similar to Case E. In this case, the occurring cracking is scarce during both the excavation and the heating phase, and is located in close proximity to the tunnel perimeter.
Figure 5-15. Microcracking and temperature evolution during the heating phase, Case F2.
Figure 5-16. Microcracking around the TSX chamber due to the excavation (closed circles) and heating (open circles). Simulation Case F2.

Because of the significant differences in the damage occurring in the cases B, C, F2 and E, G2, a new simulation case was created. The main factor affecting the occurring of damage is the strength of the PFC2D material. In the models listed above, the material strengths varied by a factor of two. Case H was similar to cases G2 and F2, except that the material strength was set to 1.5 times the material strength of the ‘base’ case B. The overall behavior of Case H was similar to the previous cases, and accordingly, more damage was observed in the roof region than at the floor, as shown in Figures 5-17 and 5-18. As expected, the range of the damage’s amount and extent was between the two end cases. The damage did not extend beyond 1 meter from the tunnel wall, nor was there a clear notch type formation visible. Case
J, the behavior of which is shown in Figures 5-19 and 5-20, is practically the same as Case H, but with wall servo controls engaged throughout the simulation.
Figure 5-17. Microcracking and temperature evolution during the heating phase, Case H.
Figure 5-18. Microcracking around the TSX chamber due to the excavation (closed circles) and heating (open circles). Simulation Case H.
Figure 5-19. Microcracking and temperature evolution during the heating phase, Case J.
Case K revisits Case F2 with the full wall servo control engaged. The resulting damage and temperature evolution are shown in Figures 5-21 and 5-22. The other comparable case is Case C, with the only difference being the heating mechanism. The behavior is similar to those cases. There is a clear notch type formation at the roof, as well as suppressed damage at the floor. It seems, however, that in Case K the difference between the roof and floor damage is not that well defined. Comparison between the simulation cases shows that the varying material strength is the main contributing factor determining the extent of the damage. Another, less important factor is the heating mechanism. All cases show the effect of the confinement at the floor level by a restrained damage below the tunnel. Based on the
simulation cases with coarse PFC2D specimen, Case J was chosen to be created as the fine resolution model and is presented in Section 5.7.
Figure 5-21. Microcracking and temperature evolution during the heating phase, Case K.
Figure 5-22. Microcracking around the TSX chamber due to the excavation (closed circles) and heating (open circles). Simulation Case K.
5.6.2 Seismic response

At set time intervals, the seismic P wave velocities were measured in the PFC2D specimens. The raypath location was chosen so that it could be related to the in-situ TSX data. Figure 5-7 shows the two raypaths in the TSX experiment that were chosen for comparison. They are located farthest from the clay bulkhead. One raypath is aligned sub-horizontally below the floor, the other in the sidewall. Unfortunately, there was no raypath coverage in the roof region, where most of the damage occurred. Measurement of the wave velocities in PFC2D, which was based on the work by Hazzard & Young (2004), was described in Section 4.2.3. The raypath in the PFC2D TSX models was oriented horizontally, at a depth of about 1.2 meters below the tunnel floor. In the measurement routine, the right-hand particle (‘pulser’) was displaced horizontally; the following response field traverses the specimen, and is monitored by the left-hand particle (‘receiver’). The input wave amplitude was set to 1.0, and the frequency to 2500 Hz. These values were chosen so that the expected wavelength would be at least 10 particles long. The input values are dependent on the PFC specimen’s particle size; the smaller the particles, the higher the input frequency. Section 4.2.4 provided a sensitivity analysis of the factors that are affecting the wave velocity measurements. Travel time, and thus the corresponding velocity, is calculated from the first peaks of the waveforms. The raypath used in the TSX simulations and sample waveforms are shown in Figure 5-23.
Figure 5-23. Seismic velocities were measured below the chamber floor, replicating the location of the in-situ data. The waveforms displayed in the graph show the horizontal movements of the pulser and receiver particles with time.

The measurements were taken at five specific points in time during the simulation: the initial stressed state, after the excavation, and after 1, 4 and 12 weeks of heating. The measured P wave velocity value for the initial state was 6120 m/s. Figure 5-24 shows the measured wave velocity changes from the initial value. In some cases, the value seems to be unusually high when compared to the general trend. These cases exhibit extensive and localized damage that produces high stress concentrations which are then picked by the velocity measurement. The overall noticeable trend is that the final velocity is less than it was in the virgin state. This makes sense because in the virgin state, neither the chamber nor any damage was present.
Some of the cases, however, do not follow this trend. One reason for this is that the excavation increases stresses around the chamber, which would, without extensive damage, be manifest as increased velocities.

Figure 5-25 shows the change of the velocities as compared to the velocity recorded after the excavation. The graph omits any measured values in between the various time periods at which measuring occurred, and shows only the final changes. The velocity recorded after the excavation stage varied for each case, and was found to be ranging from 6080 to 6120 m/s. After 12 weeks of heating, the value of the recorded changes varied from decreasing by 30 – 70 m/s to increasing by 100 m/s in Case K, and increasing up to 400 m/s in Case F2. What the two higher end cases have in common is the extensive damage in the floor area, as compared to those cases in which a general decreasing trend of the velocity value was observed. The more intense and notch-shaped floor damage produced intensified stresses below the floor, which had a direct impact on the measured velocities. The other cases had sparse microcracking in the floor area, which manifested itself as lower velocities. In those cases, the damage was not large enough to produce significant stress increase and thus higher velocities. In general, damage could lead to higher stresses on the local level, and thus higher velocities; but since the cracking simultaneously decreases the velocities, in total this effect could remain invisible to the velocity measurements.

The accuracy of some of the velocity measurement is debatable. It appeared that the combination of the close proximity between the tunnel void and the raypath on the one hand, and relatively large particle sizes on the other might have affected the results. Less than 10 particles separated the tunnel floor and the raypath. In addition, the noise arising from the
constantly moving particles (as noted in Section 4.2.3) resulted in a situation where the measurement procedure’s auto-picking routine picked erroneous peaks in some of the waveforms, thus producing incorrect velocity values.
Figure 5-24. Seismic velocity changes from the initial (pre-excavated) stage.
5.7 Comparison with TSX data

This section presents the comparison of the PFC2D simulation results with the data from the Tunnel Sealing Experiment. The model used was a simplified representation of the complex long-term underground in-situ experiment, which included excavation, filling, pressurization, and heating stages. Including the 1-year heating phase, the experiment ran a total of 7 years. In the model, only the excavation, filling, and heating steps were implemented, and were simulated for the relatively short period of 12 weeks. It was therefore not expected that the model would present all the features observed in-situ. However, it was expected that some of the key features, such as the effect of the filling material on the damage development, would
be observed during the simulations. Another comparison parameter was the temperature evolution around the chamber. In addition, the seismic velocities were measured during the simulation, and subsequently compared to the in-situ velocity data.

The damage, based on the TSX microseismic data, extended about 1.5 meters from the tunnel walls. Figure 5-26 presents the distance distributions of the TSX MS events as well as PFC2D microcracks for the Cases C and J. It was calculated that 95% of the events would occur within a range of 1.4 meters from the walls. About 85% of the events were located less than a meter from the walls. For all the PFC2D simulation cases, 70 - 100 % of all cracks occurred less than 1.0 meter from the walls. The microseismic events from the TSX data were filtered to only include events from a one-meter slice in the middle of the chamber. The PFC2D model represented a 2D slice of the chamber. In what follows, two selected cases from the simulations are compared to the TSX data. Case C represents the upper end case, and Case J represents the lower end. The main differences in the model input parameters are the material strength as well as the employed heating mechanism. The material used in Case J is 1.5 times stronger than the material in Case C. In Case C, only the center particles were heated. Case J, on the other hand, also included heating of the tunnel perimeter particles.
Figure 5-26. Distribution of the damage from the tunnel wall. Data from TSX (left) and PFC2D simulation Cases C (top right) and J (bottom right).

The damage was divided into two time-slices; damage that occurred after the excavation but before the heating, and damage directly related to the heating. Visual comparisons between
the in-situ results and the simulation results are presented in Figures 5-27 and 5-28. These figures represent the cases C and J, respectively. After the excavation stage, only a few cracks are apparent in the stronger material used in Case J. The simulation results exhibit an obvious increase of the damage during the heating phase. In Case C, a clear notch-type damage formation was observed at the roof level. The TSX data exhibits subtler notch formation, but it is clear that the damage is concentrated in the roof region. For Case J, the visual difference between the roof and floor damage is less evident; the numerical data (Figure 5-19), however, makes it apparent that there is more damage in the roof region than there is in the floor region. The damage at the floor is sparse, as opposed to the roof region, where the cracking is concentrated near the chamber’s center axis. The roof damage is similar to that of the TSX experiment. The in-situ stresses were slightly inclined in the TSX tunnel, which is manifest in the rotated damage formation around the chamber. The stresses in the PFC2D simulations were oriented perpendicularly along the horizontal and vertical axes.
Figure 5-27. Damage around the TSX chamber after the excavation phase (top) and after the heating phase (bottom). TSX in-situ MS data (left), and the PFC2D microcracks of the simulation Case C (right).
Figure 5-28. Damage around the TSX chamber after the excavation phase (top) and after the heating phase (bottom). TSX in-situ MS data (left) and the PFC2D microcracks of the simulation Case J (right).
During the PFC2D simulations, the temperature was monitored in eight locations, namely four locations along a horizontal line and four locations along a vertical line, with both lines extending from the center of the chamber. All locations show consistently rising temperatures during the heating stage. Figure 5-29 shows the temperature graphs measured near the sidewall for the cases C and J, as well as the temperature data from the TSX, which was measured inside the rock mass near the chamber. In Case C, the heating was applied to particles inside the chamber, while in Case J, the perimeter particles were heated. In Case J, the temperature monitoring location was therefore in close proximity to the heated particles, and shows as a more rapidly rising temperature curve when compared to Case C. Overall, the temperature evolution nevertheless compares satisfactorily with the in-situ data. Note that the initial temperature was set to 10°C in the models, while the ambient temperature in the TSX rock mass was about 14°C.
Figure 5-29. Temperature development during 12 weeks of heating, measured at the sidewall for models C and J, and near a TSX chamber (in borehole PZ17T) in the experiment.

The velocity data from the TSX experiment covered a region below the chamber floor, situated near the clay bulkhead. The raypath P3-R4 was aligned sub-horizontally below the chamber floor, while the raypath P3-R16 traversed almost vertically at the side of the tunnel, but still below the floor. Both raypaths are shown in Figure 5-7. For comparison with the PFC2D simulation, a comparable model raypath was chosen. Figure 5-30 presents the velocity changes during the heating phase for the PFC2D simulation Cases C, J and K, as well as the TSX data from the first 3 months of the heating phase. The measured velocity changes in the simulation cases do not perfectly fit with the in-situ data. The main reason for
the deviation is the fact that the in-situ velocities are not affected by the thermal cracking near the chamber. Furthermore, the model raypaths are situated slightly closer to the chamber than the in-situ raypaths. The increasing velocities trend observed in-situ contributed to the stress increase from the heating. The behavior of the TSX velocity data can be explained as follows: the occurring thermal stresses were closing the existing microcracks in the walls, as compared to the floor region, where the cracks were mostly closed prior to the heating phase, simply by the built-up pressure from the filling material (Collins et al, 2003). A PFC model, on the other hand, does not have any pre-existing cracks. In the simulation, the thermal stresses do not seem to close the few excavation microcracks enough to produce the same effect. On the contrary, in the PFC2D simulations the microcracking in the floor area increases during the heating phase, and in most cases is interpreted as a decreasing wave velocities trend. An increase in the velocity was observed for the cases F2 and K, and was attributed to the notch-shaped cracking pattern at the floor level. It concentrated higher stresses below the notch apex through which the velocity was measured. For comparison, Figure 5-31 shows the forces resulting from the floor damage as observed in Case J (no increase in velocity) and Case K (increase in velocity).
Figure 5-30. $P$ wave velocity changes during the heating phase; TSX data (top) and PFC2D data for cases C, J and K (bottom).
Figure 5-31. Damage and forces below the floor for PFC2D Cases J (top) and K (bottom) after 12 weeks of heating. The lines (magnitude scales with line width) depict the contact and bond forces between the particles. Note the force concentration in the Case K.
Another factor affecting the detailed damage formation is the particle packing of a PFC2D specimen. During the specimen generation, the model is populated with randomly located particles. Therefore, two models that vary only with regard to particle packing would yield slightly different microscopic behavior. In order to verify this for TSX simulations, Case K was simulated using five different PFC2D specimens, each of which had different particle packing characteristics. Figure 5-32 shows the damage formation after 12 weeks of heating for the three re-run models, as well as for the ‘original’ Case K model. Note how sensitive the microcracking behavior is to the initial particle packing; all other initial and boundary properties are the same for all the models. This is one of the key properties of the PFC modeling method, which provides natural heterogeneity in the modeling studies. The macroscopic mean behavior is similar in all cases, although the exact locations of the individual microcracks vary notably.

In addition to changing particle packing, one specimen was created with smaller particle size, and the simulation Case J was re-run based on these modifications. The fine resolution model had four times more particles than the coarse model (76000 and 19000, respectively). In the coarse model, the particle size was half of that in the coarse model. All other model properties were similar to the previously run modeling cases, and are described in Section 5.5. The results show that the behavior of the coarse and fine resolution models is similar, as shown in Figure 5-33. Both models exhibit more damage at the roof region than below the floor. The temperature evolution is the same in both models, and as expected, the thermal routines are not dependent on the particle size. It should be noted that reducing the particle size by about 50% does not affect the overall damage formation pattern, but provides slightly more detailed insight in the damage locations. The major difference between the fine and
coarse model cases is the computational runtime. The coarse model simulation was completed in a day, while the fine resolution model took about 10 days to finish, using a PC with a 2.66 GHz CPU.

Figure 5-32. Microcracking around the TSX chamber as a result of the excavation (closed circles) and heating (open circles) processes. Simulation Case K with modified, random particle packing.
Figure 5-33. Top: Microcracking and temperature evolution during the heating phase. Bottom: Microcracking locations in the excavation phase (closed circles) and heating phase (open circles). Simulation Case J fine. Inserts reproduce the graphs from Figures 5-19 and 5-20 for the coarse Case J.
5.8 Summary of TSX simulations

Despite the rather simple PFC2D models, the simulation responses satisfactorily captured the first order effects from the complex in-situ experiment. The damage difference between the floor and the roof regions was clearly evident in the model responses, and corresponded well to the in-situ data. The suppressed floor damage was arrested by the weight of the filling material. The confinement of only about 100 kPa was enough to effect a difference. Several parameters that were present in the in-situ experiment, such as the time-dependent damage and the pressurization of the chamber during the heating phase, were not taken into account in the simulations. It was suggested by Collins et al. (2003) that the pressurization of the chamber prevented the time-dependent cracking. This might explain why consideration of stress-corrosion routines and pressurization was not necessary in order to capture the simulated damage patterns. A summary of the capabilities and restrictions of representing the TSX in-situ experimental features in the used PFC2D models is presented in Table 5-4.

Table 5-4. Matrix summarizing the observations of the TSX simulations.

<table>
<thead>
<tr>
<th>Modeling Case TSX feature</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F2</th>
<th>G2</th>
<th>H</th>
<th>J</th>
<th>K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Damage at floor</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Damage at roof</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Extend of damage</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Pressurized fluid</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Seismic velocity changes</td>
<td>Down</td>
<td>Down</td>
<td>Down</td>
<td>Down</td>
<td>Up</td>
<td>Down</td>
<td>Down</td>
<td>Down</td>
<td>Down&amp;Up</td>
</tr>
<tr>
<td>Time-dependent damage</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Best matches</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The large-scale modeling case simulated the Tunnel Sealing Experiment, in which a section of a tunnel was filled with sand, sealed at both ends, pressurized, and heated for a year. The PFC2D models replicated a central plane-strain section of the TSX chamber. The model incorporated excavation, filling, and heating stages from the experiment. The filling material caused a differential damage to be formed around the opening, with more damage concentrating in the roof section. This first-order observation was captured in all of the slightly varying PFC2D models of the TSX case. In the experiment, about 85% of the damage occurred in a distance of less than 1.0 meter from the chamber wall. In the PFC2D models, about 78% of the cracks were confined to a region of the same distance from the chamber wall. The experimental temperature evolution around the heated chamber was compared with the simulated data, and was found to produce similar results.

The wave velocity measurements were conducted horizontally below the tunnel floor, and the experimental as well as simulated data concerning the heat-induced change in the velocity was compared. The behavior of the wave velocities measured from the models varied to a certain extent between the different cases. In general, the velocity change did not follow the same trend as observed in the in-situ experiment. Possible reasons for this deviation were elaborated in Sections 5.6.2 and 4.2.4. Also, the floor damage produced either stress intensification (thus increasing velocities) or stress decrease (hence velocity decrease), depending on the shape of the damaged region in the modeling cases. This effect was amplified in the simulation, because in the 2D model, the raypaths could not pass the cracked region from the side (out-of-plane). A full 3D model with fine sized particles might have solved these issues relating to the seismic wave propagation.
As discussed earlier in this chapter, during the analysis of the simulation results from the TSX modeling, it was observed that the velocity measurements do not match with the experimental data. In the experiment, the filling and heating processes caused the existing cracks to close in the vicinity of the floor, and thus increased the measured velocity values. A PFC model, however, does not perfectly replicate crack closure, and thus cannot produce the increasing velocities trend observed in-situ. By default, unlike real rock a PFC model does not display any cracks prior to the beginning of the simulation. In the course of the simulation, only new cracks can form (and later close). One possible way of getting around this problem is to delete a certain amount of the particle bonds in the initial PFC material, and thus create a synthetic rock sample with existing microcracking.
6 CONCLUSIONS AND RECOMMENDATIONS

Until now the PFC modeling code lacked extensive validation studies of the thermo-mechanical behavior. The thesis is the answer for that. It presents modeling studies that were conducted in order to verify and validate the bonded-particle modeling method.

This dissertation compares coupled thermo-mechanical numerical simulations with existing experimental data, and to builds confidence in the modeling method used. The validation of the code was performed with three case studies which varied from laboratory to field scales. The models were generated using PFC2D and PFC3D software. Experimental and simulated seismic data was used for the qualitative and quantitative comparisons.

On the laboratory scale, two-dimensional models were generated to study fracture initiation and propagation in a heated granite cylinder. Thermal routines developed during the simulations were then applied in the three dimensional laboratory scale models for the heated granite cube simulations. The numerical specimens were generated with particle clusters, attempting to replicate some of the microstructural features of real rock. The insights gained in these simulations were then applied to the large-scale model, which simulated a complex underground heated experiment.

6.1 Laboratory scale PFC2D study

Readily available experimental data from an old but well-defined laboratory experiment was used to parameterize PFC2D model to simulate a heated granite cylinder. The cylinder geometry allowed the simulations to be performed in 2D. The actual experiment had interesting features, such as hoop stress-induced main fracture, and analyzed AE data. At the
time of the simulation there were no published research using a similar approach. During the heated cylinder modeling, few parameter studies were conducted: a study of the size of the cylinder, the sensitivity of the borehole setup (filled/empty) and a variation of the thermal and mechanical properties of the models. It is concluded that the first thermal simulation study using the bonded-particle modeling approach replicated closely the interesting aspects observed during the laboratory experiment.

The study of the development of the AE events during the numerical simulations and the laboratory experiments yielded similar results, both in fracture behavior and magnitude ranges. The laboratory AE data showed a number of trends observed in the models:

- Initial scattered microcracking,
- Microcracking propagating outwards from the central borehole (in models with a filled borehole),
- Microcracking propagating inwards from the perimeter was observed in the other models.

The models captured the behavior of the laboratory experiment, i.e. the macroscopic tensile failure driven by high hoop stresses in the perimeter of the specimen. The thermo-mechanical bonded-particle models were not able to produce cracking during the cooling of the heated specimen. More complex particle shapes could be used to replicate this behavior. Particle clusters would also enhance the mechanical response of the numerical models, as was shown in some previous studies. It is thought that the concept of non-spherical particle shapes is the future for the bonded-particle modeling method. The concept is indeed currently (2008) being developed by other researchers.
6.2 Laboratory scale PFC3D study

The second modeling study used the data from a non-complex and well-defined laboratory experiment. The data included detailed mapping of the thermal-induced cracks in grain-scale showing that majority of the cracks was occurring in grain boundaries. The size of the experimental specimen allowed the modeling study to be conducted in three-dimensions without extensive simulation time. Main part of the modeling study concentrated on the development of the enhanced particle clustering routines. The routines were then tested, and applied to thermo-mechanical models generated with PFC3D. The novel approach used breakable particles clusters to study the thermal damage in heated cubic specimens.

In the simulation the PFC3D specimens, each having about 10000 breakable particle clusters, were heated up to a temperature of 450°C. Heating-induced damage was observed by AE monitoring and P wave velocity measurements which was compared against the laboratory data. It was shown that the simulation data followed the experimental data:

- P wave velocity decrease with rising temperature up to 250°C,
- Cluster boundary cracking during the heating phase similar to the grain boundary cracking in rock samples.

Parameter study was also conducted to assess the sensitivity of the P wave measurement input parameters to the measured wave velocities.

6.3 In-situ scale PFC2D study

The third modeling study used the data from a multi-staged in-situ experiment. The experimental geometry allowed 2D modeling to be performed on the large-scale tunnel.
Seismic data from the experiment was readily available for comparison. The PFC2D models combined bonded-particles to represent the hard rock and loose particles to represent the sand filling. The simulations took account the in-situ stresses, gravity and the heating of the chamber. The conducted parameter studies showed the sensitivity of the particle packing to the formed microcracking, also the effect of the particle size was studied.

The large tunnel scale models captured the first order phenomena observed in-situ, i.e. the difference in the damage occurring in the roof and floor regions. In the experiment, the tunnel opening was filled with sand, while loose PFC2D particles were used in the models. The free particles applied a pressure of about 100 kPa to the floor area, which was enough to suppress significant amounts of damage in that region during the heating of the tunnel. Simulation cases with intense and notch-shaped floor damage produced intensified stresses below the floor, which had a direct impact on the measured velocities. In some other cases, the sparse microcracking in the floor area manifested itself as lower velocities. The damage was not concentrated enough to produce a significant stress increase, and thus did not result in higher measured velocities. In general, damage could lead to higher local stresses (which would result in higher velocities). However, the cracking simultaneously decreases the velocities, so that the total effect could remain invisible to the velocity measurements. The temperature evolution sufficiently corresponded with the in-situ data.

6.4 Recommendations

The main obstacle in large-scale thermo-mechanical modeling is the resolution, or particle size, of the models. Current computing resources (PC with 3.0GHz CPU) impose time limits on the maximum amount of particles (in the order of hundred thousands) used in the models,
and is directly related to particle size. Developments in the computational resources will make it possible to run in-situ scale simulations with millions of particles. This limited scale validation work supports the future modeling studies.

Parallelized thermo-mechanical model is currently (2008) being tested on a supercomputer in the Rock Fracture Dynamics Laboratory at the University of Toronto. It permits PFC3D models with millions of particles. The approach can be used to construct realistic tunnel scale models. The use of particle clusters, in size of a grain, will permit simulations and direct quantitatively comparisons with the laboratory data, for example with crack density values. The smaller particle size is hypothesized to overcome deficiencies found during the research presented in this thesis. The large three-dimensional models would produce full AE fingerprints, which would facilitate comparison with experimental seismic data. Figure 6-1 shows two models in different scales that were generated during the testing of the parallelized PFC3D.

Another future development area is to take account fluids in the thermo-mechanical bonded-particle models. Laboratory experiments usually assume dry conditions hence the hydro mechanics is not major factor in the laboratory scale simulations. However the fluid part becomes more important when dealing with wet underground cavities. Some of the other observations made in the simulations carried out for this thesis, such as the inability of the models to produce seismicity from the fracture surfaces shearing against each other, will require more fundamental changes to the current modeling routines.
Figure 6-1. Left – 30 cm sided rock block model (1.6 million particles) heated from a central borehole. Right – Section of a 4.5 mm x 3.4 mm model with grain-scale sized particle clusters.
7 REFERENCES


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8 APPENDICES

The section presents the main developed and modified routines. This is not comprehensive listing of the codes. In order to run the actual models the used needs to include also the appropriate library files in PFC.

Codes for running numerical experiment in Section 4.1

Filename: sTSb_therMech.DVR

; created May 2005 by Toivo Wanne
; modified June 09, 2005 by TW
;
; - scaling pbond strenhths
; - introducing outer boundary temperature to simulate room temp (thermC.dat)
; - thermal cycling commands were extracted to separate driver file (June 9)
;
set logfile sTSb_tCmD15.log
set log on

new

; ..........................................................
restore sTSb_mB15-spc.sav
;SCALE PBOND STRENGHTS
SET md_scale_fac=0.6
md_scale_strengths ; => material mD
; ..........................................................

;load support functions ==================
call %itascaFishTank%FishPfc\md\fishcall.FIS ;call FISHCALL support
call %itascaFishTank%FishPfc\md\crk.FIS ;load cracking functions
call thermalSupport.fis ;load thermal support functions
call ae2002_2d.FIS ;load AE monitoring functions
call thermC.dat ;load thermal properties and introduce particle groups
; ..........................................................

;setup thermal support, monitoring and plotting
SET tf_nummeas=7 ; number of measurement circles created in earlier steps
tf_setup
tf_plotviews1
tf_plotviews2
prop xdisp=0.0 ydisp=0.0
; ..........................................................
; add histories
thermal_time ;active time tracking
his id=100 thermal_time
his id=101 ball temp 25.0e-3,0.0
his id=102 ball temp 50.0e-3,0.0
his id=103 ball temp 100.0e-3,0.0
his id=104 ball temp 145.0e-3,0.0

his id 1000 dia muf

his id=200 crack_density

;create plot view for histories
plot create temp_histories
plot add his 101 102 103 104 vs 100
plot set title text 'Temperature histories'
;-------------------
plot create crack_history
plot add his 1
plot set title text 'Crack density and number of cracks'
;-------------------

;setup AE monitoring
set ae_svel = 3000 ;shear wave velocity
set ae_Q = 100 ;quality factor

set thermal off mech on
ae_init

; SAVE STATE============
SET md_run_name='sTSb_mD15_tE'
title 'sTSa_mD15_tE'
SET md_tag_name = 'expA';initialized state and ready to thermal cycling
md_save_state

set log off
;===================================
set logfile sTSb_mD15_tE.log
set log on

;COUPLED THERMO-MECHANICAL CYCLING
;remove zap balls functionality
set fishcall 0 remove tf_zap_heater_balls

def tf_heat_it4
;input: heat_targetTemp, heat_tempInterval
  tf_AvgHeaterTemp
  _heat_currentTemp=AvgBall_temp

  loop while 1#0
    _heat_currentTemp=_heat_currentTemp+heat_tempInterval
    command
      THERM APPLY deltemp=heat_tempInterval range group HEATER_BALLS
      SET therm on mech on
      prop xdisp=0.0 ydisp=0.0
      pr @ _heat_currentTemp

      thermal fix temperature range group HEATER_BALLS
      set add_time=120 ;2 minutes
      solve ratio=1e-5 time=@th_time2
      thermal free temperature
    endcommand
  if _heat_currentTemp >= heat_targetTemp then
    exit

end_if
endloop
end

;COUPLED THERMO-MECHANICAL HEATING

set heat_targetTemp=200.0 heat_tempInterval=10.0
tf_heat_it4 ;call this function after FIRST complete thermal cycling
thermal fix temperature range group HEATER_BALLS
thermal fix temperature range group OUTER_BALLS

;Heating  
set thermal on mech on
thermal set substep 100

set add_time=3600 ;1 hours
solve ratio=1e-5 time=@th_time2

SET md_tag_name = 'expDm_ae'
md_save_state

;Cooling  
:free temperature fixity flag for all particles
thermal free temperature
:and fix temp of outer balls (=room temp) before continuing
thermal fix temperature range group OUTER_BALLS

;let heat flow in the sample without heating
set add_time=3600 ;time for thermal calculation, additional 1 hour
solve ratio=1e-5 time=@th_time2 ;this command uses total thermal time

SET md_tag_name = 'expDm_ae'
md_save_state

set log off
return

Filename: tf.FIS  Support functions for Thermal Problems
;modified March 8 2005 by TW
;=================================================================================
;
; 12 May 2005 temperature contour plot option added
;
;=================================================================================
def tf_setup
;
crk_init
command
history reset
history nstep=20
history id=1 crk_num ; cracks that have formed
end_command
;
loop _i (1, tf_nummeas)
  _hisxx = 10*_i + 1
  _hisyy = 10*_i + 2
  _hisxy = 10*_i + 3
command
.history id=@_hisxx measure s11 id=@_i
.history id=@_hisyy measure s22 id=@_i
.history id=@_hisxy measure s12 id=@_i
end_command
end_loop
end
;=================================================================================
def tf_avg_stresses
;
; ----- Return the average stresses based on all meas circles.
;
; INPUT: tf_nummeas
; OUTPUT: tf_avg_s{xx,yy,xy}
;
  cnt = 0
  tf_avg_sxx = 0.0
  tf_avg_syy = 0.0
  tf_avg_sxy = 0.0

loop _mid (1, tf_nummeas)
  mp = find_meas(_mid)
  jj = measure(mp, 1); compute stress for this meas-circle
  cnt = cnt + 1
  tf_avg_sxx = tf_avg_sxx + m_s11(mp)
  tf_avg_syy = tf_avg_syy + m_s22(mp)
  tf_avg_sxy = tf_avg_sxy + 0.5*(m_s12(mp) + m_s21(mp))
end_loop

if cnt > 0 then
  tf_avg_sxx = tf_avg_sxx / cnt
  tf_avg_syy = tf_avg_syy / cnt
  tf_avg_sxy = tf_avg_sxy / cnt
else
  tf_avg_sxx = 0.0
  tf_avg_syy = 0.0
  tf_avg_sxy = 0.0
end_if
end

;==============================================
def tf_plotviews1
  command
    plot create mechanical_system
    plot set title text & 'Mechanical system.'
    plot add ball yellow
    plot add wall black
    plot add disp blue

    plot create model_system
    plot set title text & 'Model system.'
    plot add group lorange red
  end_command
end
;==============================================
def tf_plotviews2
  command
    plot create thermal_system
    plot set title text & 'Thermal system.'
    plot add ball yellow
    plot add wall black
    plot add pipe blue
    plot add temp red scale=2e-2
    plot add power black
  end_command
end
;==============================================
def thermal_time
  thermal_time = th_time
end
;==============================================
def th_time2
;
; ----- INPUT: th_time - current accumulated thermal time
; ; add_time - additional time for heating/cooling
;
th_timecurrent=th_time
th_time2=th_time+add_time

end

;========================================
def tf_minerals

;ID of minerals
ID_mineAlower=1
ID_mineAupper=int(mineA*md_numballs)

ID_mineBlower=ID_mineAupper+1
ID_mineBlower=int(mineB*md_numballs)+ID_mineBlower

ID_mineClower=ID_mineBlower+1
ID_mineCupper=int(mineC*md_numballs)+ID_mineClower+10

command
set safe_conversion off
range name MineralA id ID_mineAlower,ID_mineAupper
range name MineralB id ID_mineBlower,ID_mineBlower
range name MineralC id ID_mineClower,ID_mineCupper

group MineralA range MineralA
group MineralB range MineralB
group MineralC range MineralC
set safe_conversion on
endcommand

end

;========================================
def tf_AddIDsToArray

;add heater balls (a named group) ball pointers to array list

;default named group 'HEATER_BALLS', not (yet) an input parameter
;output: number of balls in the list 'num_heaterBalls'

array HeaterB_IDs(500)

bp=ball_head
num_heaterBalls=0
loop while bp # null
    dummy=inrange('HEATER_BALLS',bp)
    if dummy = 1 then
        num_heaterBalls=num_heaterBalls+1
        HeaterB_IDs(num_heaterBalls) = (bp)
    end_if
    bp = b_next(bp)
end_loop

;tf_AddIDsToArray

;=================================================================================
def tf_AvgHeaterTemp

;average temperature of heater balls

SumBall_temp = 0.0
nn = 0
loop nn (1,num_heaterBalls)
    th_bp = (HeaterB_IDs(nn))
    ball_temp1 = b_thtemp(th_bp)
    SumBall_temp = SumBall_temp+ball_temp1
end

end_loop
AvgBall_temp = (SumBall_temp/num_heaterBalls)
end

;=================================
;zap balls
;function that deletes balls that are detached
;only balls that belong to named group 'HEATER_BALLS' are considered

def tf_zap_heater_balls

while_stepping

zap_del_count = zap_del_count + 1
if zap_del_count > 99 then
    zap_del_count = 0
    zap_numballs = 0

    bp = ball_head

    loop while bp # null ;--------
        next = b_next(bp)

        if inrange('HEATER_BALLS',bp) = 1 then
            if md_numtcon_bp < 1 then
                ii = b_delete(bp)
                zap_numballs=zap_numballs+1
                tf_AddIDsToArray
            end_if
        end_if
        bp = next
    end_loop ;-------------------
end_if
end

;========================================

def tf_heat_it

;input: heat_targetTemp, heat_tempInterval

_heat_currentTemp=20.0

loop while 1#0

_heat_currentTemp= _heat_currentTemp+heat_tempInterval
command
    THERM APPLY deltemp=@heat_tempInterval range group HEATER_BALLS
    SET therm off mech on
    prop xdisp=0.0 ydisp=0.0
    pr @_heat_currentTemp
    solve ratio 1e-8
endcommand

if _heat_currentTemp >= heat_targetTemp then
    exit
end_if
endloop
end

;========================================

def tf_heat_it2

;input: heat_targetTemp, heat_tempInterval

tf_AvgHeaterTemp

_heat_currentTemp=AvgBall_temp
loop while 100

    _heat_currentTemp=_heat_currentTemp+heat_tempInterval
    command
        THERM APPLY deltemp=@heat_tempInterval range group HEATER_BALLS
        SET therm off mech on
        prop xdisp=0.0 ydisp=0.0
        pr @_heat_currentTemp
        solve ratio 1e-5 ;time=@th_time2
    endcommand

    if _heat_currentTemp >= heat_targetTemp then
        exit
    end_if

endloop
end

;++++++++++++++++++++++
def tf_pi_cylinder
; circle plot item to add in various plots

plot_item
    Array _tf_pt1(dim)
    stat= set_line_width(0)
    stat= set_color( 0 )
    ;origin of a cirle
    _tf_pt1(1) = 0.0
    _tf_pt1(2) = 0.0
    _tf_rad = (0.5*et2_xlen)
    stat = draw_circle( _tf_pt1, _tf_rad )
end

;++++++++++++++++++++++
def crack_density
; added June 9, 2005
; calculates crack density of the model

; area must be circular with diameter equals to et2_xlen
; otherwise this must be modified
    area = (0.5*et2_xlen)*(0.5*et2_xlen)*pi
    crack_length = md_ravg*2
    sum_length=crack_length*crk_num
    crack_density = sum_length/area
end

;=================================================================================
; Contour temperatures
; modified by TW, 13 May 2005
;=================================================================================
def col_default
    _my_max = -1.0e20
    _my_min = 1.0e20
end
def my_colors
; -- First find max and min ball temperature ...
    _my_range = _my_max - _my_min
    _max_temp = -1.0e20
    _min_temp = 1.0e20
    _b_pnt = ball_head
loop while _b_pnt # null
_bid = b_id(_b_pnt)
_max_temp = max(_max_temp,b_thtemp(_b_pnt))
_min_temp = min(_min_temp,b_thtemp(_b_pnt))
_b_pnt = b_next(_b_pnt)
end_loop

_min_t = _min_temp
_max_t = _max_temp

if _my_range = -2.0e20 then
  _t_range = _max_temp - _min_temp
else
  _max_temp = _my_max
  _min_temp = _my_min
  _t_range = _max_temp - _min_temp
endif

_col_dt = _t_range/40.0
_min_temp = _min_temp - _col_dt*0.5

; --- Next assign ball color code according to its temp ...

_b_pnt = ball_head
loop while _b_pnt # null

  _bid = b_id(_b_pnt)
  _b_cindx = int((b_thtemp(_b_pnt) - _min_temp)/_col_dt)
  b_color(_b_pnt) = _b_cindx
  _b_pnt = b_next(_b_pnt)
end_loop

command
group _con1 ran color 0 15
group _con2 ran color 16 31
group _con3 ran color 32 41
end_command
end

;-----------------------------------------------
def _chg_cid

  ; --- Because we can only display 16 colors per plot item, 
  ; we must re-assign ball color ids in each group to 
  ; reflect this fact ...
  _bpt = ball_head

  loop while _bpt # null

    if b_color(_bpt) > 15 then
      if b_color(_bpt) < 32 then
        b_color(_bpt) = b_color(_bpt) - 16
      endif
    endif

    if b_color(_bpt) > 31 then
      b_color(_bpt) = b_color(_bpt) - 32
    endif

    _bpt = b_next(_bpt)
  end_loop
end

;-----------------------------------------------
def make_tcview

  if _tc_tcviewexists = 1 then
    tc_destroy_tcview
  endif

end

;-----------------------------------------------
def tc_destroy_tcview

  if _tc_tcviewexists = 1 then
    command
      plot cur 0
    plot destroy temp_contour
  end_command
  _tc_tcviewexists = 0
end

;-----------------------------------------------
def makeTempCont

command

    make_tcview
    _col_default
    _my_colors
    _chg_cid

macro c1  'rgb 1.00 0.00 0.00'    ; red
macro c2  'rgb 1.00 0.10 0.00'
macro c3  'rgb 1.00 0.20 0.00'
macro c4  'rgb 1.00 0.30 0.00'
macro c5  'rgb 1.00 0.40 0.00'
macro c6  'rgb 1.00 0.50 0.00'
macro c7  'rgb 1.00 0.60 0.00'
macro c8  'rgb 1.00 0.70 0.00'
macro c9  'rgb 1.00 0.80 0.00'
macro c10 'rgb 1.00 0.90 0.00'
macro c11 'rgb 1.00 1.00 0.00'    ; yellow
macro c12 'rgb 0.90 1.00 0.00'
macro c13 'rgb 0.80 1.00 0.00'
macro c14 'rgb 0.70 1.00 0.00'
macro c15 'rgb 0.60 1.00 0.00'
macro c16 'rgb 0.50 1.00 0.00'
macro c17 'rgb 0.40 1.00 0.00'
macro c18 'rgb 0.30 1.00 0.00'
macro c19 'rgb 0.20 1.00 0.00'
macro c20 'rgb 0.10 1.00 0.00'
macro c21 'rgb 0.00 1.00 0.00'    ; green
macro c22 'rgb 0.00 1.00 0.10'
macro c23 'rgb 0.00 1.00 0.20'
macro c24 'rgb 0.00 1.00 0.30'
macro c25 'rgb 0.00 1.00 0.40'
macro c26 'rgb 0.00 1.00 0.50'
macro c27 'rgb 0.00 1.00 0.60'
macro c28 'rgb 0.00 1.00 0.70'
macro c29 'rgb 0.00 1.00 0.80'
macro c30 'rgb 0.00 1.00 0.90'
macro c31 'rgb 0.00 1.00 1.00'    ; turquoise
macro c32 'rgb 0.00 0.90 1.00'
macro c33 'rgb 0.00 0.80 1.00'
macro c34 'rgb 0.00 0.70 1.00'
macro c35 'rgb 0.00 0.60 1.00'
macro c36 'rgb 0.00 0.50 1.00'
macro c37 'rgb 0.00 0.40 1.00'
macro c38 'rgb 0.00 0.30 1.00'
macro c39 'rgb 0.00 0.20 1.00'
macro c40 'rgb 0.00 0.10 1.00'
macro c41 'rgb 0.00 0.00 1.00'    ; blue

macro _bc3 'c9 c8 c7 c6 c5 c4 c3 c2 c1'
macro _bc2 'c25 c24 c23 c22 c21 c20 c19 c18 c17 c16 c15 c14 c13 c12 c11 c10'
macro _bc1 'c41 c40 c39 c38 c37 c36 c35 c34 c33 c32 c31 c30 c29 c28 c27 c26'

    pl cre temp contour
    pl ad bal _bc1 range group _con1
    pl ad bal _bc2 range group _con2
    pl ad bal _bc3 range group _con3
endcommand

end
ret

Filename: thermC.DAT
config thermal
THERM PROP sheat=1015. ; exp=3.711e-6

;identify three sets of particles and assign different expansion coeffs.
set mineA = 0.30 ;Quartz
set mineB = 0.40 ;Plagioclase
set minec = 0.70 ;1.00-(mineA+mineB) ;Muscovite/biotite

tf_minerals
THERM PROP exp=25.0e-6 range group MineralA ;quartz
THERM PROP exp=15.0e-6 range group MineralB ;palgioclase
THERM PROP exp=10.0e-6 range group MineralC ;biotite

;-----------------------------------------------------------
THERM MAKE conductivity 3.5 measure 5
THERM INIT temp=20.0

;=================================================================
;identify heater particles around center hole
range name HEATER_BALLS circle cen 0,0 rad 18.0e-3
range name OUTER_BALLS circle cen 0,0 rad 147.0e-3

;identify outer particles around specimen
range name OUTER_BALLS circle cen 0,0 rad 147.0e-3

return

def _more_arrays
array out_string(1)
end

Filename: Bond_forces.FIS

def pBond_forces
    _fn = string(md_run_name)+string(md_tag_name)+'.txt'
    stat = open(_fn,1,1)
    cp = contact_head ;pbond associated with contact
    loop while cp # null
        pbh = c_pb(cp) ;pbond address
        if pbh # null then
            out_string(1) = string(pb_nforce(pbh))+string(pb_sforce(pbh))
            stat = write(out_string,1)
        end_if
        cp = c_next(cp)
    end_loop
    stat = close
end
pBond_forces
return

Codes for running numerical experiment in Section 4.2

;Example used in the BPM course project
;created 29/11/2004 by TW
;
%modified December 8th 2006
%clustering study

; Westerly granite clustered specimen

;-----------------------------
restore s3ECl_mC36ae-spc.SAV

; delete flying particles (outside a 50mm$^3$ box)
del ball range x -25.0e-3 25.0e-3 y -25.0e-3 25.0e-3 z -25.0e-3 25.0e-3 not

;set echo off
call %itascaFishTank%
  FishPfc
  md
  fishcall.FIS  ;call FISHCALL support
call %itascaFishTank%
  FishPfc
  ae2004_3d.FIS ;load AE monitoring functions

set ae_svel = 3000 ;shear wave velocity
set ae_Q = 100 ;quality factor

; make clustered specimen
call cluster.FIS

set extra ball 3
set cl_size 7
set cl_bslt 3
cl_conglomerate

; create plots ===========================
; pl create cluster
; pl add fish cl2_pi1 bl blu green cyan red magenta orange brown yellow

; apply cluster strengths =============
set md_clusters = 1

; intracluster
SET pb_sn_mean=320e6  pb_sn_sdev=74e6
SET pb_ss_mean=320e6  pb_ss_sdev=74e6

; intercluster
SET pb_sn_mean_btn=160e6  pb_sn_sdev_btn=36e6
SET pb_ss_mean_btn=160e6  pb_ss_sdev_btn=36e6

md_pbprops

solve ratio 1e-5

set echo on
SET md_run_name='s3ECl_mC36ae'
  SET md_tag_name = 'cluster'
  md_save_state  ;=> *.*.SAV

Return

; Filename: cluster.FIS

; PURPOSE: Functions to create clusters of particles such that different
; properties can be assigned within and between the clusters.
;
; Itasca Consulting Group, Inc.

; Modified by TW
; June 14, 2006 - [_cl_forall_bp1] b_type -> pointer_type

def cl_arrays
  Array _cl_pt0(dim)
end
def cl_conglomerate

Generate a conglomerate (a rock composed of fragments varying from pebbles to boulders held together by a cementing material) by starting with the current assembly that is assumed to be densely packed and identifying arbitrarily shaped clusters of balls. We attempt to maximize the number of balls in each cluster subject to the constraint that no cluster contains more than [cl_size] balls.

A cluster is defined as a set of balls that are adjacent to one another where adjacent means that a connected path can be constructed between any two balls in a cluster by traversing ball-ball non-virtual contacts.

The clusters are identified using the b_extra(bp, [cl_bslt]) variable. The algorithm uses the b_extra(...) fields to designate:
- 0 - unmarked
- i>0 - w/i cluster-i

Upon algorithm completion, there will be no unmarked balls remaining.

**USAGE:**
1) SET EXTRA ball <ival0> ; ival0 > 0
2) cl_size = <ival1>
   cl_bslt = <ival2> ; ival2 <= ival0
   cl_conglomerate

**INPUT:** cl_size - maximum number of balls in each cluster
cl_bslt - slot in b_extra( bp, [cl_bslt] ) to be used

**OUTPUT:** cl_num - total number of clusters formed

**EFFECTS:** modifies the b_extra(bp, [cl_bslt]) FISH variable

```fish
_cl_clear_marks
_cl_num = 0
bp = ball_head
loop while bp # null
  if b_extra( bp, cl_bslt ) = 0 then
    md_stk_init
    cl_num = cl_num + 1
    _cl_cnt = 0
    _cl_addbp = bp
    _cl_add ; {i: _cl_addbp}
    section
      loop while 1 # 0
        bp1 = md_stk_pop
        if bp1 = null then ; empty stack
          exit section
        end_if
        _cl_forall_bp1
        ;
        if _cl_cnt = cl_size then ; cluster filled
          exit section
        end_if
      end_loop ; while 1 # 0
    end_section
    end_if
  bp = b_next(bp)
end_loop
md_stk_clear ; to eliminate possible dangling pointers
end
```

---

```python
plot_item

--- Plotitem for visualizing clusters by placing filled circles in ball centroids with circle color based on cluster number.

**INPUT:** cl2_pi1_fac - multiplication factor for icon sizes (default: 1.0)
```
if cl2_pi1_fac = 0 then  
c12_pi1_fac = 1.0  
end_if

bp = ball_head
loop while bp # null
  _cl_pt0(1) = b_x(bp)
  _cl_pt0(2) = b_y(bp)
  if dim = 3 then
    _cl_pt0(3) = b_z(bp)
  end_if
  _rad = cl2_pi1_fac * b_rad(bp)
  _cindex = b_extra(bp, cl_bslt)
  stat = set_color(_cindex)
  stat = fill_circle(_cl_pt0, _rad)
  bp = b_next(bp)
end_loop
end

----
Plotitem for visualizing clusters by drawing filled circles
(of color-1) at contacts within clusters and (of color-2)
at contacts between clusters.

; INPUT: cl2_pi2_fac - multiplication factor for icon sizes (default: 1.0)

if cl2_pi2_fac = 0 then  
c12_pi2_fac = 1.0  
end_if

cp = contact_head
loop while cp # null
  if cl_internal_cp = 1 then
    stat = set_color(0)
  else
    stat = set_color(1)
  end_if
  _cl_pt0(1) = c_x(cp)
  _cl_pt0(2) = c_y(cp)
  if dim = 3 then
    _cl_pt0(3) = c_z(cp)
  end_if
  _avgrad = 0.5 * (b_rad(c_ball1(cp)) + b_rad(c_ball2(cp))
  _rad = cl2_pi2_fac * _avgrad
  stat = fill_circle(_cl_pt0, _rad)
  cp = c_next(cp)
end_loop
end

----
Returns as a boolean indicating whether given contact [cp]
is internal to a cluster. Return value = 1-is internal;
2-btm. two clusters.

; INPUT: cp - contact pointer

cl_internal_cp = 0
if md_cbond = 0 then
  if md_pbond = 0 then ; it is not a bonded contact, exit
    exit
  end_if
end_if
if b_extra(c_ball1(cp),cl_bslt) = b_extra(c_ball2(cp),cl_bslt) then
  cl_internal_cp = 1
end_if
end

def cl_numclusters
  ; ----- Returns the total number of clusters in the model.
  ;
  ; INPUT: cl_bslt - slot in b_extra( bp, [cl_bslt] ) where cluster-info is
  ;
  _maxclnum = 0
  bp = ball_head
  loop while bp # null
    _clnum = b_extra( bp, cl_bslt )
    _maxclnum = max( _maxclnum, _clnum )
  bp = b_next(bp)
  end_loop
  cl_numclusters = _maxclnum
end

def cl_numwi
  ; ----- Returns the number of bonds (either contact or parallel) that are
  ;       within clusters.
  ;
  ; INPUT: cl_bslt - slot in b_extra( bp, [cl_bslt] ) where cluster-info is
  ;
  _numwi = 0
  cp = contact_head
  loop while cp # null
    _bonded = 0
    if md_cbond = 1 then
      _bonded = 1
    end_if
    if md_pbond = 1 then
      _bonded = 1
    end_if
    if _bonded = 1 then
      if cl_internal_cp = 1 then
        _numwi = _numwi + 1
      end_if
    end_if
  cp = c_next(cp)
  end_loop
  cl_numwi = _numwi
end

def cl_numbtn
  ; ----- Returns the number of bonds (either contact or parallel) that are
  ;       between clusters.
  ;
  ; INPUT: cl_bslt - slot in b_extra( bp, [cl_bslt] ) where cluster-info is
  ;
  _numbtn = 0
  cp = contact_head
  loop while cp # null
    _bonded = 0
    if md_cbond = 1 then
      _bonded = 1
    end_if
    if md_pbond = 1 then
      _bonded = 1
    end_if
    if _bonded = 1 then
if cl_internal_cp = 0 then
  _numbtn = _numbtn + 1
end_if
end_if

cp = c_next(cp)
end_loop

cl_numbtn = _numbtn
end

;================================================================================
def _cl forall_bp1
  ;;
  ;; Loop over all balls adjacent to bp1, add unmarked ones to the
  ;; current cluster. Break out of this function when either:
  ;; (1) all adjacent balls have been visited, or
  ;; (2) cluster has been filled.
  ;;
  ;; if _cl_cnt = cl_size then ; cluster filled
  ;;  exit
  ;;
  ;; cp = b_clist(bp1)
  loop while cp # null
    if c_nforce(cp) # 0.0 then ; not a virtual contact
      if b_type(c_ball2(cp)) = 0 then  ; THIS WORKS IN OLD pfc VERSION
        if pointer_type(c_ball2(cp)) = 100 then  ; it is a ball-ball contact,
          if c_ball1(cp) = bp1 then
            bp_other = c_ball2(cp)
          else
            bp_other = c_ball1(cp)
          end_if
        else
          bp_other = c_ball1(cp)
        end_if
      end_if
    end_if
    if c_ball1(cp) = bp1 then
      cp = c_b1clist(cp)
    else
      cp = c_b2clist(cp)
    end_if
  end_loop
end

;================================================================================
def _cl clear_marks
  ;
  ;; bp = ball_head
  loop while bp # null
    b_extra( bp, cl_bslt ) = 0
    bp = b_next(bp)
  end_loop
end

;================================================================================
def _cl add
  ;
  ;; Add ball [_cl_addbp] to current cluster and push onto stack.
  ;;
  ;; INPUT: _cl_addbp
  ;;
  ;; b_extra( _cl_addbp, cl_bslt ) = cl_num
  ;; _cl_cnt = _cl_cnt + 1
  ;; md_stk_item = _cl_addbp
  ;; md_stk_push
  end

;================================================================================
return
; Example used in the BPM course project
; created 29/11/2004 by TW
;
; modified December 11th 2006
; clustering study
;
; --------------------------------------------
restore s3EC1_mC36ae-cluster.SAV
;
; set echo off
;
; call cluster grouping functions
call cl_ArrayShuffling_dev.FIS
;
; divide clusters to N groups
set cl_Ngroups = 3
cl_grouping
;
; create plot
pl create groups
pl add group
;
; ------------------------------------------
Return
;
; Routines to identify cluster groups with a given size
; created September 15, 2006 by TW
;
; mod 20/9/2006 by TW: added link to workign shuffle FISH functions
;
; file includes various grouping routines developed during the work
;
; set array size
def cl_arraysize
cl_arraysize = cl_numclusters ; set here number of clusters
end cl_arraysize
;
; declare array and initialize to zero
def cl_initarray
array cl_cluster_IDs(cl_arraysize)
loop j (1, cl_arraysize)
   cl_cluster_IDs(j) = 0
endloop
end cl_initarray
;
; fill array with cluster IDS (i.e. integers from 1 to number of clusters)
def cl_addIDsArray
loop j (1, cl_arraysize)
   cl_cluster_IDs(j) = j ; cluster IDS go from 1 to cl_arraysize
endloop
end cl_addIDsArray
;
; shuffle cluster ID array to random order
call shuffle.fis ; cl_cluster_IDs and cl_arraysize need to be defined before shuffle
;
; assign balls to cluster groups (named range)
def cl_grouping
  _subN = round(cl_numclusters/cl_Ngroups)
; loop through balls
bp=ball_head
loop while bp # null
   ballID = b_id(bp)
   _clnum2 = (b_extra( bp, cl_bslt )); get cluster ID# of ball bp
   ; find matching group in cluster ID array
   loop J(1,cl_arraysize)
      tempJ = cl_cluster_IDs(J)
      if tempJ = _clnum2 then
         ii=OUT(string(j))
         _cl_assignGroupname
      end_if
   endloop
   bp = b_next(bp)
end_loop
end

; assign groupname to a particle corresponding to cluster ID in [cl_grouping]
; support function
def _cl_assignGroupname
   ; input: J - index of cluster ID in array
   ; match J to ID range
   ; assign corresponding group name
   ;[range name grouptitle id @_ballID]
   ;[group grouptitle range grouptitle]
   loop try(0,cl_Ngroups)
      arrayIDrange = _subN*try
grouptitle = 'group_'+string(try)
      if J > arrayIDrange then
         command
            range name grouptitle id @_ballID
            group grouptitle range grouptitle
         endcommand
      endif
   endloop
end
ret

; end of file

; SHUFFLE FISH function
; shuffle functions to FISH (PFC)
; created on 19/9/2006 by TW
; final version 20/9/2006

; INPUT:
; cl_cluster_IDs - array containing IDS
; cl_arraysize - size of the array containing IDS

;====== SHUFFLE WITH SWAP ===============
;main function for shuffling
def shuffle
   cl_randomseed
   loop k (1,cl_arraysize) ;loop through cluster ID array
      cluster_ID = cl_cluster_IDs(k) ;get cluster ID
      _cl_random
      cluster_ID_random = cl_cluster_IDs(cl_random)
      swap ;swap values from k'th place to random place
      ;ii=out(cl_cluster_IDs(k))
   endloop
end

;swap k'th cluster ID with a random ID from cl_random'th place
def swap
   _temp = cluster_ID

cl_cluster_IDs(k) = cluster_ID_random
cl_cluster_IDs(cl_random) = _temp
end

; provide a random number between k'th and cl_arraysize
def _cl_random ; have to be different name than function inside!!
  _min = k
  _max = cl_arraysize-1
  _tempW = (_max - _min + 1)
  cl_random = round(urand*_tempW) + _min
end

def cl_randomseed
  _randomseed = round(clock)
  ; randomseed should be close to 10000 so here is a rude checking routine
  if _randomseed < 1000 then
    _randomseed = _randomseed * 10
  end_if
  if _randomseed > 50000 then
    _randomseed = _randomseed/10
  end_if
  if _randomseed > 100000 then
    _randomseed = _randomseed/100
  end_if
  command
    set random _randomseed
  endcommand
end

def cl_printout
  loop kk (1,cl_arraysize)
    _cl_temp = cl_cluster_IDs(kk)
    ii=out(_cl_temp)
  endloop
end

; shuffle
; ============================== end of SHUFFLE WITH SWAP ===============================

Filename: Heat_s3EC1_mC36ae.DVR

; modified December 14th 2006
; clustering study
;
; HEATED SPECIMEN (ARBITRARY PACKING) three cluster groups
; with different thermal coefficients
; ----------------------------------------------------------
; APPLY deltemp DEGREES CELSIUS in specimen
; ----------------------------------------------------------
restore ../s3EC1_mC36ae-relaxed.SAV

set echo off

call %itascaFishTank%\FishPfc\md\crk.FIS
set echo on

crk_init
ac_init

set log on

CONFIG therm

; from Yingwei Fei
THERM PROP exp=10.0e-6 range group group_0 ;microcline
THERM PROP exp=5.0e-6 range group group_1 ;plagioclase
THERM PROP exp=25.0e-6 range group group_2 ;quartz
THERM PROP exp=5.0e-6 range group group_3 ;unite with group_1

THERM INIT temp=0.0

call ..\\HeatingSupport.fis

; add histories
his id 101 crk_num
his id 201 ae_num
his id 202 aec_num

thermal_time ;active time tracking
; his id 500 thermal_time
his id 501 ball temp 0.0 0.0 0.0

-------------------
set heat_targetTemp=450 heat_tempInterval=5
heat_it

title 's3ECl_mC36ae, plus 450C'

SET md_tag_name = 'sTSX_mLdBA-\plus450nw'
md_save_state ; => *.SAV

set log off

return
:fname: Heat_s3ECl_mC36ae.DVR

Codes for running numerical experiment in Chapter 5

; (specimen & material parameters)
; new => **{nn} - {bal,pck,iso,flt,spc}
;
; last mod. TW 27-Sep-07
; TSX rectangular specimen for heated experiment

set logfile sTSX_mLdBA-spc.log

set log on

new
set safe_conversion on

set gen_error off

SET disk on ; model unit-thickness cylinders
SET echo off ; load support functions
call %itascaFishTank%FishPfc-md\md.FIS

call %itascaFishTank%FishPfc2-et2\et2.FIS

call %itascaFishTank%FishPfc\md\flt.FIS

SET echo on

call mA-\param.DAT
SET md_run_name='sTSX_mA1'
title 'sTSX_mA1'

SET random 10002
SET et2_rlo=0.07
SET tm_numtries=250000

; rectangular
SET et2_ylen=21.0 et2_xlen=28.0
SET et2_prep_saveall=0
et2_prep

; clean up: delete flying particles
del ball range x @_xl,@_xu not
del ball range y @_yl,@_yu not
pr md_numballs

; modify existing meas circles
meas id 1 rad 6.5
meas id 2 rad 6.5
meas id 3 rad 6.5

set log off

; ===========================================================================
return

Filename: TSX_stresses.DAT, Triaxial-Test Control Parameters
;
; last mod. TW Oct-10-2007
; ===========================================================================
set logfile TSX_mLdA-si.log
set log on
call %itascaFishTank%\FishPfc\md\fishcall.FIS

SET et2_knxfac=1.0 et2_knyfac=1.0
; define stresses (at walls)
SET et2_wsxx_req=45e6
SET et2_wsyy_req=11e6

SET et2_ws_tol=0.01
SET p_sr=1.0  p_cyc=400  p_stages=10
et2_pvel
et2_wallstiff
et2_seatbiax
et2_sample_dimensions

SET md_tag_name = '-si'
md_save_state
set log off

; ===========================================================================
return

Filename: TSX_thermal.DVR
; created September 2007 by Toivo Wanne
; mod November more histories, refined stress values (not in this file)
; case K

set logfile TSX_thermal_K.log
set log on
; load support functions

; modify existing meas circles
meas id 1 rad 6.5
meas id 2 rad 6.5
meas id 3 rad 6.5
;------------------------
; change pbond strengths
;SET md_scale_fac=1.5
;md_scale_strengths
;------------------------
; setup thermal, monitoring and plots

call thermalSupport.FIS

config thermal
THERM PROP exp=10.0e-6 ;isotropic
THERM PROP sheat=1015.0
THERM MAKE conductivity 3.5 measure 2
THERM INIT temp=10.0

range name OUTER_BALLS x -13.5 13.5 y -10 10 ;28x21m
group OUTER_BALLS range OUTER_BALLS not
thermal fix temperature range group outer_balls

set thermal on mech off
step 5 ;initialize,

; create additional meas circles
meas id 10 x 7.0 y 9.0 rad 3.0 ; right side of the tunnel
meas id 11 x 0.0 y 7.0 rad 3.0 ; above the tunnel
; meas circle-derived stresses
history id=510 meas s11 id 10 ;xx
history id=610 meas s22 id 10 ;yy

history id=511 meas s11 id 11 ;xx
history id=611 meas s22 id 11 ;yy

;------------------------
; add histories
; history reset

history nstep=20

history id=1 crk_num ; cracks that have formed
thermal_time ; active time tracking
his id=100 thermal_time
his id=101 ball temp 0,0 ; horizontal line
his id=102 ball temp 2,0
his id=103 ball temp 3,0
his id=104 ball temp 4,0
his id=105 ball temp 5,0
his id=106 ball temp 6,0 ; vertical line
his id=202 ball temp 0,2
his id=203 ball temp 0,3
his id=204 ball temp 0,4
his id=205 ball temp 0,5
his id=206 ball temp 0,6

;average stresses (overlap the tunnel void)
history id=113 et2_msxx
history id=114 et2_msyy

history id=13 et2_wsxx ; wall-derived stresses
history id=14 et2_wsyy

his id 1000 dia muf

; create plot view for histories
plot create temp_histories_X
plot add his 101 102 103 104 105 106 vs 100
plot set title text 'Temperature histories, horizontal'

plot create temp_histories_Y
plot add his 101 202 203 204 205 206 vs 100
plot set title text 'Temperature histories, vertical'

plot crack_history
plot add his 1
plot set title text 'Number of cracks'

plot wall_stress_hist
plot add his 13 14
plot set title text 'Stress histories @ walls'

plot meas_stress_hist
plot add his 510 511 610 611
plot set title text 'Stress histories @ meas circles'

;"define heater element"
SET ce_A=2.40 ce_B=2.1

plot in_heater range fish elli_element

;"excavate"
SET ce_A=2.20 ce_B=1.88
plot in_ellips range fish elli_element

prop pb_n 0.0 range group in_ellips ; TSX chamber
set mech on ther off
cy 5
ini rad mul 0.995 range group in_ellips
set grav 0 -9.81
crk_init ;start microcrack monitoring

cy 5

solve ratio 1e-5 ;if lower will 'never' reach equilibrium

SET md_tag_name = '-excavated'
md_save_state

;remove wall servo controls ==> walls fixed
;set et2_servo_xon = 0
;set et2_servo_yon = 0

; heating. also the filling material
THERM APPLY deltemp=75.0 range group in_heater
thermal fix temperature range group in_heater

THERM APPLY deltemp=75.0 range group in_ellips
thermal fix temperature range group in_ellips

prop xdisp=0.0 ydisp=0.0

; solve coupled T-M
SET therm on mech on
thermal set substep 100

; ONE WEEK ****************************
solve ratio 1e-5 time=604800 ; one week

SET md_tag_name = '-1week_TMs'
md_save_state
; AFTER 4 WEEKS ***********************
solve ratio 1e-5 time=2419200 ; 4 weeks

SET md_tag_name = '4weeks_TMs'
md_save_state

; AFTER 12 WEEKS ***********************
solve ratio 1e-5 time=7257600 ; 12 weeks

SET md_tag_name = '12weeks_TMs'
md_save_state

;===================================
set log off
return
;EOF: