Study of Mechanical and Flow Properties of Weakly Cemented and Uncemented Sands Using a Discrete Element Method

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Study of Mechanical and Flow Properties of Uncemented and Weakly Cemented Sands Using a Discrete Element Method

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Abstract

Many natural gas and oil reserves are situated in uncemented and weakly cemented formations. These formations exhibit different mechanical and transport properties compared to cemented, consolidated ones. Phenomena such as sand production, wellbore stability, subsidence and permeability alteration during production have been reported in field experience and in numerous experimental results. Our work is intended to analyze these issues.

A two dimensional discrete element method is developed using the commercial software PFC-2D, with the aim of studying the mechanical and transport properties of uncemented and poorly cemented sandstones. Unconfined compressive tests of poorly cemented sands, triaxial, hydrostatic compressive and radial extension tests of cemented and uncemented materials were simulated. Failure modes under different conditions and the effect of micromechanical properties of the rock’s constituents on the macroscopic behavior were studied. Comparison of our simulations to the experimental data was used to reaffirm the validity of the DEM method we are using. Pore collapse is observed in hydrostatic compression tests of weakly bonded sands with a critical pressure of 17 MPa. The failure mechanism of weakly cemented sands during triaxial tests changes at a critical confining pressure of about 4 MPa from brittle failure to strain thickening ductile failure.

Using a pore network fluid flow model which takes into account the mechanics of the material from a microscopic point of view, permeability variation with deformation
during triaxial, radial extension and hydrostatic compression tests was simulated and the results shown. The permeability of uncemented and weakly cemented sands is dependent on the stress state of the system and the stress path followed. Permeability of uncemented sands decreases by 55% at 5.4 MPa hydrostatic stress and by 35% before shear failure in triaxial tests of 1.0 MPa confining pressure. It increases up to 200% of the initial value during shear failure in 0.35 MPa confining stress triaxial tests and up to 200% during radial expansion tests. Weakly cemented sands’ permeability drops by 60% at 19 MPa hydrostatic pressure. Pore collapse which occurs at 17 MPa hydrostatic pressure speeds up the irrecoverable reduction in permeability. A 60% reduction in permeability of weakly cemented sands is also observed during 1.5 MPa confining pressure triaxial tests. Weakly bonded samples’ vertical permeability increases by 200% during radial expansion tests with an initial hydrostatic pressure of 5.0 MPa. A strong coupling between permeability evolution and stress-deformation state of the system exists and is confirmed in the results of all tests simulated.
### TABLE OF CONTENTS

1 Introduction and Background ............................................................................. 11
   1.2 Literature Review ......................................................................................... 14
   1.3 Objective .................................................................................................... 18
2 Discrete Element Method Model ........................................................................ 20
   2.2 Contact Model ............................................................................................. 21
      2.2.1 Force Displacement law: ......................................................................... 22
      2.2.2 Bonding .................................................................................................. 25
   2.3 Fluid Flow Formulation .............................................................................. 28
3 Mechanical Test Simulations ............................................................................. 33
   3.1 Sample Preparation ..................................................................................... 33
   3.2 Choosing the micromechanical parameters ............................................. 37
   3.3 Hydrostatic Compression Tests .................................................................. 51
   3.4 Unconfined Compressive Tests on Weakly Bonded Samples ..................... 54
   3.5 Triaxial Tests .............................................................................................. 60
      3.5.1 Compressive Triaxial Tests ................................................................. 62
      3.5.2 Effect of Confining Pressure during Conventional Triaxial Test .......... 66
   3.6 Radial Expansion Failure Simulations: ...................................................... 69
4 Permeability Variation Simulations ................................................................... 74
   4.1 Procedure .................................................................................................... 74
   4.2 Choosing the fluid flow micro properties ................................................. 77
   4.3 Permeability variation with initial porosity ............................................. 80
   4.4 Permeability Variation due To Hydrostatic Stress ...................................... 82
   4.5 Permeability Variation during Triaxial Tests ............................................ 86
   4.6 Permeability Variation during Failure due to Decreasing Confining Stress 96
5 Summary ........................................................................................................ 103
6 Bibliography .................................................................................................... 109
7 Appendix .......................................................................................................... 112
FIGURES AND TABLES

Figure 2.1: Calculation cycle (from Itasca, 2001)..................................................................22
Figure 2.2: Ball-Ball contact (from Itasca 2001).................................................................23
Figure 2.3: Ball-Wall contact (from Itasca 2001).................................................................23
Figure 2.4: Illustration of the Bond, Forces and Moments associated with it. Itasca 2001. .27
Figure 2.5: Pore and pore throat geometry. The white lined polygons denote a ‘pore’ and
the green lines the ‘pore throat’ network connecting the pores centers which are the
green dots....................................................................................................................29
Figure 2.6: Pore pressure forces on the particles. .................................................................32
Figure 3.1: Particle radius probability distribution. .............................................................35
Figure 3.2: Balls and compression forces between them after the balls have moved and
unbalanced forces are sufficiently low. This is the stage when the balls are bonded
and friction is activated .............................................................................................35
Figure 3.3: Balls and compression forces after the walls are removed and the sample is
allowed to expand for a cemented material case. As seen the force chains between
the balls change after the sample is relaxed..............................................................36
Figure 3.4: Grain-Cement-Grain System from Potyondy and Cundall 2004. .......................38
Figure 3.5: Isotropic stress at the end of sample generation procedure of the unbonded
sample as a function of initial 2-D porosity......................................................................44
Figure 3.6: Triaxial test of unbonded samples with different particle Young’s moduli.
Confining stress is 0.35 MPa for all tests. ......................................................................45
Figure 3.7: Unbonded sample's macroscopic Young's modulus' dependence on the
particles’ Young modulus. .........................................................................................45
Figure 3.8: Triaxial tests of unbonded samples with different friction coefficient. Confining
stress is 0.35 MPa for all tests. .....................................................................................46
Figure 3.9: Dependence of triaxial differential strength of unbonded samples on the value
of friction coefficient.................................................................................................46
Figure 3.10: Unconfined compressive tests of bonded samples with different bond
strengths. 2-D porosity is 0.15 and the bond size multiplier is 1.0...............................47
Figure 3.11: Unconfined strength of bonded samples with different bond strength. 2-D
porosity is 0.15 and the bond size multiplier is 1.0.....................................................47
Figure 3.12: Unconfined strength of bonded samples with different bond strength. 2-D
porosity is 0.15 and the bond size multiplier is 1.0.....................................................48
Figure 3.13: Dependence of UCS on the bond size multiplier Lambda. .............................48
Figure 3.14: Hydrostatic stress versus volumetric strain during hydrostatic compression of
unbonded sample. ......................................................................................................53
Figure 3.15: Hydrostatic stress versus volumetric strain during hydrostatic compression test
of weakly bonded sample. ............................................................................................53
Figure 3.16: Evolution of broken bonds with volumetric strain starting at 2.5% strain value till the end of loading stage of the test. Blue is tension induced broken bonds and red is shear induced broken bonds.

Figure 3.17: Compressive stress versus strain in an unconfined compressive stress of a weakly bonded sample.

Figure 3.18: Broken bond configuration on the weakly bonded sample at different equally spaced axial strain values, starting from 1.5% strain till the end of the test at 6.8% strain value. Blue is tension induced broken bonds and red is shear induced broken bonds.

Figure 3.19: Unconfined compressive strength versus 2-D porosity for bonded samples.

Figure 3.20: Macroscopic Young's modulus versus porosity for bonded samples during unconfined compressive tests.

Figure 3.21: Differential stress (top), radial and volumetric strain (bottom) versus axial strain during a triaxial test on an unbonded sample. The confining stress is 0.35 MPa.

Figure 3.22: Differential stress (top), horizontal and volumetric strain (bottom) versus axial strain during a triaxial test on a weakly bonded sample. The confining stress is 0.35 MPa.

Figure 3.23: Differential stress versus axial strain during triaxial tests of different confining pressures of unbonded samples.

Figure 3.24: Shear stress versus average normal stress at failure during triaxial tests for unbonded samples.

Figure 3.25: Differential stress versus axial strain during triaxial tests of different confining pressures of weakly bonded samples.

Figure 3.26: Broken bonds of the same weakly bonded sample after failure during triaxial tests. The confining stress was 0.5 MPa for the left and 6.0 MPa for the case on the right.

Figure 3.27: Vertical and horizontal stresses, volumetric and horizontal strain versus radial (horizontal) strain during a radial expansion test on an unbonded sample. The initial hydrostatic stress is 1.5 MPa.

Figure 3.28: Vertical and horizontal stresses, volumetric and horizontal strain versus radial (horizontal) strain during a radial expansion test on a weakly bonded sample. The initial hydrostatic stress is 15.0 MPa.

Figure 4.1: Pressure profile on x-direction permeability measurement simulations.

Figure 4.2: Detail on how the flow rate through a line (black) along the sample is measured. Flow rates through all the pore throats which cut the black line (surrounded by the blue rectangles) are added for the calculation of permeability.

Figure 4.3: Permeability Variation with the parameter C1. The gap multiplier parameter C2 is set to 1.0. The hydrostatic stress is 1 MPa.

Figure 4.4: Effect of gap multiplier C2 on the permeability. C1 is set to 0.15. The hydrostatic stress is 5 MPa.

Figure 4.5: Permeability versus initial bonded sample porosity. The samples were under 1.0 MPa hydrostatic stress.
Figure 4.6: Permeability variation of an unbonded sample under hydrostatic compression test. Ko=249 D.................................................................84
Figure 4.7: Permeability variation of a weakly bonded sample under hydrostatic compression test. Ko=8.48 D.........................................................85
Figure 4.8: Permeability variation with hydrostatic stress for the two types of samples ....85
Figure 4.9: Normal contact force chain for an unbonded sample under 0.5 MPa (left) and 5 MPa (right) hydrostatic stresses........................................86
Figure 4.10: Permeability variation (bottom) and differential stress (top) versus axial strain of an unbonded sample during 0.35 MPa confining stress triaxial test. ...............91
Figure 4.11: Permeability variation (bottom) and differential stress (top) versus axial strain of an unbonded sample during 1.0 MPa confining stress triaxial test. .............92
Figure 4.12: Permeability variation (bottom) and differential stress (top) versus axial strain of a weakly bonded sample during 0.35 MPa confining stress triaxial test..............93
Figure 4.13: Particles and broken bonds, normal force chains and pore throat network for the bonded sample at the beginning of the low confining stress (1 MPa) triaxial sample and at the end of it..........................................................94
Figure 4.14: Permeability variation (bottom) and differential stress (top) versus axial strain of a weakly bonded sample during 1.5 MPa confining stress triaxial test..............95
Figure 4.15: Permeability variation (bottom) and stresses (top) versus horizontal strain of an unbonded sample during radial expansion test. Initial hydrostatic stress is 1.5 MPa.................................................................99
Figure 4.16: Permeability variation (bottom) and stresses (top) versus horizontal strain of an unbonded sample during radial expansion test. Initial hydrostatic stress is 5.0 MPa.................................................................100
Figure 4.17: Permeability variation (bottom) and stresses (top) versus horizontal strain of a weakly bonded sample during radial expansion test. Initial hydrostatic stress is 5.0 MPa.................................................................101
Figure 4.18: Permeability variation (bottom) and stresses (top) versus horizontal strain of a weakly bonded sample during radial expansion test. Initial hydrostatic stress is 15.0 MPa.................................................................102
1 Introduction and Background

1.1 Introduction

Computation models of rocks’ mechanical and transport properties may be classified into two major groups: continuum models and discrete element models. In continuum models the material and its properties are mathematically dealt with as a continuum; mechanical damage and failure is modeled indirectly as a change in the applied constitutive relationships between stress and strain. The same is valid for the transport properties and the coupling between the fluid pressure and flow and the mechanics of the material. There are several constitutive relationships which relate permeability, porosity and the stress state on different types of rock (Bouteca et al. 2000).

The discrete element models’ approach on the other hand is more direct; it idealizes the material as a collection of structural units (beams, particles or disks) bonded together at their contact points. The breaking of these bonds, due to exceeding forces or stresses acting at the local structural level represents the damage and failure. Most structural engineering applications use the continuum models whereas when a study of tracking and evolution of the cracks within a material is needed the direct, DEM models are utilized (Cundall 2001).

Many of the mechanisms occurring in the rock are complex and difficult to characterize with the existing continuum theories. At best, in order to capture and reproduce the whole spectrum of a rock’s behavior under stress and during failing, one needs many parameters to input into the model. The difficulty stands in the fact that it’s the
mechanical microstructure which determines some of the rock’s behavior. Our model, in which the rock is approximated as a collection of bonded or unbonded particles provides a way of considering the effect of the important micro mechanisms. The length scale of the constituents is related to the particle size in clastic rocks and provides the necessary resolution needed to gain an insight into how the microstructure affects the macroscopic behavior.

Large oil and gas reserves stored in formations known as uncemented or weakly cemented are known to exist and are being produced in many areas of the world. Weakly cemented rocks show a different mechanical behavior in response to the stresses they are under, compared to well cemented rocks. They have lower shear and tensile strength and a higher compressibility than the well cemented rocks and are thus more heavily affected by the reduction of reservoir pressure, which increases the effective stresses in the reservoir. (Al Tahini et al., 2006; Abbas et al., 2002; Nikraz et al., 1999; Dautriat et al., 2007; Nicholson et al., 1998; Ruistuen et al., 1996 and Saaidi et al., 2004). There are two types of stresses acting on the pore structure in a reservoir rock: internal, due to the fluid pressure and drag, and external stresses which are a result of overlying and surrounding formations. Any change in any two types of stresses will alter the effective stresses which in turn induce strains, deformations and failure. Sand production is one of the most common and severe problems associated with poorly cemented rock failure. Sand production, which may be defined as transport of solids by the produced fluid causes severe damage to the production equipment, such as submersible pumps, plugs off the casing perforations and could eventually completely plug off the production column (Da Fontura and Dos Santos,
In addition to sand production, other problems which arise in weakly cemented and un cemented reservoirs are related to compaction and subsidence. The famous subsidence in Ekofisk field in the North Sea is believed to have occurred due to rock compaction and pore collapse of the poorly consolidated rock. (Chin and Boade, 1989). Pore collapse induced subsidence causes damage to the drilling and production equipment and may lead to very costly repairs or even abandonment of the well.

The porosity and permeability of the reservoir also change as a result of compaction, quite often damaging the productivity of a well (Davies and Davies 2000). Compaction in general narrows the pore throat openings and as a result decreases the permeability. However this effect may be overcome by the generation of cracks and fractures; channels of high fluid flow conductivity which may be oriented in a preferred direction. It has been suggested and seen experimentally that the effect of stresses on the permeability depends on the stress regime the formation is in, namely pre- and post-failure at least in the case of brittle rocks Bruno (1981), Al-Harthy (1998), Baghini (2008), Ruistuen and Teufel (1996, 1999).

During the production of the hydrocarbons from the reservoir, fluid pressure decreases, whereas the value of the external stresses remains the same. This in turn induces changes in the effective stresses of the system. Rhett and Teufel (1992) show that the ratio K of the change in horizontal stresses ($\Delta \sigma_h$) to the change in the vertical stresses ($\Delta \sigma_v$) is a constant. For this reason the value of the differential stress q increases while the pore pressure decreases. According to the poroelastic theory (Biot and Willis, 1957) with b being Biot’s poroelastic constant, and $P_p$ the pore pressure:

$$K = \frac{\Delta \sigma_h}{\Delta \sigma_v}$$
\[ \Delta q = -b(1-K)\Delta p_p \]  

It is this increase in differential stress what we are simulating with the triaxial tests. In a triaxial test vertical stress increases whereas the side (horizontal) stress is kept constant, increasing the value of the differential stress. However as Dusseault (1997), Oldakowski (1994) and Teufel (1996, 1999) have shown, the deformation and permeability evolution of a rock depends strongly on the stress path followed. For this reason we simulate radial expansion and hydrostatic mechanical and fluid flow tests as well.

1.2 Literature Review

Cundall (2001) discusses future prospects, the advantages and shortcomings of discontinuous modeling of materials based on the DEM method of Cundall and Strack (1979). As the computing power to simulate larger numbers of particles increases, DEM models are expected to have a more important role in geomechanics simulations. Examples on formulation of a bonded particle model for cemented rocks, micromechanics, tuning of the micromechanical parameters and response to triaxial and Brazilian tests on Lac du Bonnet granite are by Potyondy and Cundall (2004) and by Powrie et al (2005). Stress corrosion and cracking from a micro mechanical point of view, crack initiation and propagation were studied by Park et al (2007), Cheng et al (2003) and Cho et al (2007) developing a model with the method of circular particle clusters showed the role of crushable particles on the macroscopic behavior a material. Deposition and sedimentation histories play an important role on the properties of clastic rocks (Jin et al 2003) and

Early works on shear failure of rocks under compressive load and poroelastic properties of rocks has been done by Maurer (1965), Wilhelmi et al (1967) and by Senseny (1983). A work on sand production, wellbore stability and the effect of mechanical strength of reservoir rocks has been done by Zhang et al (2000). The effect of porosity and stresses on dilatancy has been studied by Larsen et al (1998). Saidi et al. (2005) presents a work on the mechanical properties of synthetic weakly cemented sandstones and the dependence on the amount and type of cementation. The work of Abbas et al. (2002) shows the dependence of rock strength and other mechanical properties on the phenomenon of sand production. Segall (1989) presents a work on the possibility of fluid extraction being the cause of earthquake in several major producing areas.

Soares et al. (2002) present permeability variation results during uniaxial strain experiments of limestones and unconsolidated sandstones core samples from deep water reservoirs in Campos Basin. They report pore collapse and a reduction in permeability from 120 to 10 mD for axial stresses up to 100 MPa in limestones and a reduction from 160 to 10 mD for axial stresses from 20 to 80 MPa in the permeability of friable, uncemented sands. Effects of decreasing pore pressure on sandstone samples under true triaxial stress conditions are reported by Al-Harthy et al. (1998). For a reduction in pore pressure from 14
to 1 MPa they report a maximum permeability reduction of 60-70%. Permeability evolution with pore pressure depends on the stress state of the sample with the biggest reduction in hydrostatic stress conditions. Permeability evolution with pore pressure also shows path dependency. The work of Crawford and Yale (2002) however, shows that the greatest permeability reduction occurs in nonhydrostatic loading due to pore collapse. Similar results are shown in the work of Ruistuen et al. (1996) with the biggest reduction in permeability occurring in pore pressure reduction in rocks under triaxial stress conditions. Dautriat et al. (2007) performed hydrostatic compression experiments on Bentheimer sandstone and Esteillades limestone core samples and report a 45% decrease in permeability at a maximum stress of 65 MPa for the sandstone permeability and a permeability reduction of 90% in the permeability of the limestone cores at the same maximum hydrostatic stress. Davies and Davies (2001) present a summary of field measurements and experimental data for permeability and porosity reduction due to production. Permeability may reduce up to 2 orders of magnitude in samples from Travis Peak formation due to the closure of natural fractures and microcracks under stresses. The work of Thallak et al. (1993) shows a maximum 50% permeability reduction during triaxial tests of Brady sandstone samples at a confining pressure of 35 MPa. Experience with rock compaction and reservoir performance on a North Sumatra Offshore field is described in the work of Pathak et al. (2007). They report a larger reduction in permeability (65%) in higher porosity (0.38) weak sandstone samples, compared to only a 10% decrease in lower porosity (0.16), better consolidated samples. Sarda et al. (1999) performed hydrostatic and triaxial compression experiments in Vosges sandstone samples. A reduction up to 50% in
permeability is reported during hydrostatic stresses up to 100 MPa. However permeability increases in lower porosity rocks after they fail. David et al. (1994) performed hydrostatic compression experiments on sandstones and report a change in the trend of permeability reduction at a critical pressure where pore collapse occurs. Schutjens and de Ruig (1996) report a 90% reduction in permeability of sandstone samples under uniaxial strain and hydrostatic loading experiments. An order of magnitude reduction in permeability and hysteresis on permeability evolution on Indiana Limestone samples is reported in the work of Salvadurai and Glovacki (2004). Permeability evolution in fractured media is studied in the work of Zhang et al. (2006). A 90% reduction is reported on hydrostatic loading experiments. However they also report an increase of an order of magnitude during triaxial tests. A similar increase in permeability during triaxial tests on brittle rock samples is also reported in the work of Shao et al. (2005). Permeability evolution during triaxial tests in several sedimentary rock types (mudstone, sandy shale, fine and medium sandstone) is studied in the work of Wang and Park (2002). They also report an increase of 2-3 fold increase in the permeability of these rocks after brittle failure in triaxial conditions.

The referenced experimental results show that permeability of all kinds of rocks decreases under hydrostatic loading conditions as the stress increases. The amount of diminution in the permeability depends on the porosity of the rock; the higher the porosity, the more the reduction. Permeability reduction depends also on the strength and compressibility of the rock. The more compressible, least cemented rocks’ permeability decreases at a larger extent. The amount of natural fractures and microcracks existing in the
rock also plays a role with permeability decreasing orders of magnitude under hydrostatic stresses due to closure of fractures in tight, highly compacted rocks. High porosity carbonates show a larger reduction in porosity and permeability than sandstones under hydrostatic stresses due to pore collapse.

Permeability variation under nonhydrostatic compression experiments is relatively more complicated, with several authors reporting an increase or at least a recuperation of the initial permeability after brittle failure in consolidated sandstones. In general the more brittle the failure mechanism is, the higher the permeability increase is. Ductile failure induces permeability reduction. Initial permeability and porosity also is important in permeability evolution in non-hydrostatic tests on both sandstones and carbonates. Lower initial porosity and permeability, tight rocks’s permeability increases more after brittle failure compared to high permeability, weakly consolidated rocks. Experimental results show a strong coupling of permeability with the stress-strain state of the rocks in the majority of the experiments, with transitions in the trend of variations occurring at the same point in both permeability and stress-strain state of the system.

1.3 Objective

The objective of this work is to present a working discrete element method model which allows a better understanding of the micromechanics of weakly cemented and uncemented sands’ behavior under stresses, failure modes under different conditions and
the effect of micromechanical properties of the rock’s constituents on the macroscopic behavior.

Another objective of this research is to study the coupling of transport and mechanical properties of materials under different stress states and stress paths. The effect of microscopic properties on the permeability and permeability variation with stresses under different mechanical tests is studied.
2 Discrete Element Method Model

2.1 PFC description

PFC (Particle Flow Code) is a software that models the movement and interaction of circular particles based on the Discrete Element Method (DEM) developed by Cundall and Strack (1979). A problem which involves motion and interaction between particles can be tackled using the PFC software using the correct form of interaction between the individual particles. Although the granular material seems to be PFC’s natural domain of operation, solid and brittle material may also be modeled by a proper bonding between the individual particles. The result is a solid which with the right amount and properties of bonding behaves mechanically like a solid brittle object. The variation in amount, strength and stiffness of the bonding which corresponds to different amount and quality of cementation in real rocks, together with other micro mechanical properties of the assembled sample allows to model materials with different macro mechanical properties.

Differently from continuum models, where one needs to utilize thoroughly different theoretical models to account for the behavior of different materials, the transition in the DEM method of PFC is smooth. By changing the relevant micromechanical properties one gets a different macro mechanical response. The ability to add bonds to particles is of value particularly in the case of sandstones and siliciclastics in general, where it is known that the rock we observe today is a product of diagenesis of the initially loose individual grains of sand where compaction and cementation occurs with time.
However this flexibility of the DEM method applied in PFC comes with a price. Compared to continuum models, the geometry of the problem, properties of the final solution and especially setting the boundary and initial conditions is not so straightforward. For example there is no unique way of assembling a sample of specified porosity, permeability and mechanical properties since there is no unique way to pack a great number of particles. Forces between the particles, hence stresses within the assembly and the stress boundary conditions depend on the particular packing of the particles.

2.2 Contact Model

The model used in our work is composed of distinct particles that move independently of each other (Cundall and Strack 1979). Each single particle interacts with each neighbor particle at the contact point or interface between them. The particles are treated as rigid with the contact occurring at a point. Overlap between neighboring particles can occur at the contact. The amount of overlap is dependent on the amount of the compressive and/or shear forces between the two particles. Bonds may exist between a particle and its neighbors which it shares a contact with. Our model is 2-D so the forces act on a plane (X-Y) with moments acting only about the Z-axis. No forces acting out of the plane are considered. The sample can be considered as a collection of cylinders of different diameters and unit length.

In addition to the particles which are referred to as balls in the PFC software, and bonds between them, the other element used in the model are the walls. Walls interact with balls in a fashion similar to the balls interaction between themselves. However, walls do
not interact with each other. By assigning a velocity to the walls, stress boundary conditions are obtained. Two types of contacts may exist in the model: ball-ball and ball-wall.

The equations of motion are applied to each particle until it reaches equilibrium (i.e., until forces acting on it balance to within a numerical limit). Contacts and forces associated with them may be lost and new contacts may form as the particles move (Figure 2.1).

![Diagram of calculation cycle](From Itasca, 2001)

**Figure 2.1: Calculation cycle (From Itasca, 2001)**

### 2.2.1 Force Displacement law:

The force-displacement law is the constitutive model which relates the force acting between two particles or between a particle and a wall to the relative displacement between them. The force may be decomposed into two components, the normal force, $F^n$, which acts in the direction of the normal vector, $n_l$, and the shear force, $F^s$, which acts on the tangential plane (line) at the contact. The normal vector, the contact plane and the overlap vector $U^n$ are indicated in the Figure 2.2 and 2.3.
The total force for each ball $i$ has normal and shear components,
\[ F_i = F_{i}^n + F_{i}^s, \quad (2.1) \]

where the normal force is given by

\[ F^n = K^n U^n. \quad (2.2) \]

\( K^n \) is a secant modulus in the sense that it relates total displacement/overlap, \( U^n \) with force. The value of \( K^n \) is determined by the contact stiffness model.

The shear force is set to zero when a contact is formed even if there is an overlap between particles. As particles move and slide past each other, the shear force increases incrementally each time step as

\[ \Delta F^s = -k^s \cdot \Delta U^s, \quad (2.3) \]

in which

\[ \Delta U^s = V^s \Delta t. \quad (2.4) \]

with \( V^s \) being the relative shear velocity of the particles in contact. \( k^s \) is a tangent modulus in that it relates incremental displacement/overlap \( \Delta U^s \) with increments in force.

The linear contact model, which was used in this study, is defined by the normal and shear stiffnesses \( k_n \) and \( k_s \) (with units of Force/Displacement) and the two contacting entities (ball-ball or ball-wall). The stiffnesses of the two entities A and B (ball-ball or ball-wall) are assumed to act in series. The normal stiffness is given by

\[ K^n = \frac{k_n^A k_n^B}{k_n^A + k_n^B}, \quad (2.5) \]

and similarly the shear stiffness
The normal and shear stiffness parameters $k_n$ and $k_s$ are important micromechanical parameters which determine the elastic macro properties of the system.

A factor which limits the shear force acting on the particles when sliding past each other is friction. Friction is always present in a contact when a normal compressive force exists and when there is no bonding between the two particles. When the magnitude of the shear force exceeds the maximum force of friction, the particles are allowed to slip past each other and the shear force is set to the maximum $F_{\text{max}}^s$ given by:

$$F_{\text{max}}^s = \mu |F_i^s|$$

(2.7)

The friction coefficient $\mu$ is also an important micro mechanical input that affects the behavior of the system in the macro scale.

2.2.2 Bonding

Cementation between the particles is modeled as a finite sized piece of material between two particles which establishes an elastic interaction between them. This is made possible by the incorporation of parallel bond logic in PFC (Itasca 2001). The existence of the bond does not preclude the possibility of slip. The bond can transmit both forces and moments between particles and contribute to the resultant quantities acting on them. It may be imagined as a set of elastic springs with constant normal and shear stiffnesses which are uniformly distributed over a rectangular cross section, lying on the contact plane and centered at the contact point. These springs act in parallel with the balls’ contact point.
springs. Relative motion of the bonded particles causes a force and a moment within the bond material and these forces and moments can be related to normal and shear maximum stresses at the bond periphery. If these stresses are greater than the assigned normal and shear strengths, the bond breaks. Hence, there are 5 parameters which need to be input for the bonding: normal and shear stiffnesses, $k_n$ and $k_s$, whose units are those of spring constant per bond area or stress/displacement, normal and shear strength, $\sigma_c$ and $\tau_c$, with units of stress, and bond radius $R$. 
Figure 2.4: Illustration of the Bond, Forces and Moments associated with it (Itasca, 2001).
2.3 Fluid Flow Formulation

A detailed and mechanically fully coupled model of fluid flow in discontinuous (discrete) medium would require a great computational effort. However in many cases a fully coupled and accurate approach would be unnecessary and a simpler approximate model may capture the mechanism of interest.

The fluid flow approach used in our work is a flow network model formulated by Potyondy and Cundall (1999). The elements of the network are the pores and pore throats. The fluid flows from one pore to its neighbor pore through the pore throat if there is a pressure difference between them. Since pore throats don’t actually exist in 2-D geometry for grains in contact, “notional” pore throats are created to represent the actual 3-D geometry and to give a background permeability. Thus a pore throat diameter is presumed for fluid flow even though the true distance between the particles is zero. The pores on the other hand, are defined as the smallest closed chain of particles such that each link in the chain is a contact (Figure 2.5). The pore center coordinates and pore volume are approximated using the geometry and position of its surrounding particles.

\[
x_p = \frac{1}{N} \sum_{i=1}^{N} x_i, \tag{2.8}
\]

\[
y_p = \frac{1}{N} \sum_{i=1}^{N} y_i, \tag{2.9}
\]

\[
V_p = \left( \frac{1}{N} \sum_{i=1}^{N} R_i \right) \cdot \frac{1}{N} \sum_{i=1}^{N} \left[ (x_i - x_p)^2 + (y_i - y_p)^2 \right], \tag{2.10}
\]

\[
1 \sum_{i=1}^{N} x_i = \sum_{i=1}^{N} y_i = \sum_{i=1}^{N} 1, \tag{2.10}
\]
where $x_i, y_i, R_i$ and $N$ are the x and y coordinates of the ball in the chain forming the pore, its radius and the total number of the balls surrounding the pore and $x_p, y_p, V_p$ are the coordinates and 3-D volume of the pore.

![Figure 2.5: Pore and pore throat geometry. The white lined polygons denote a 'pore' and the green lines the 'pore throat' network connecting the pores centers which are the green dots](image)

The flow through a pore throat is modeled as Hagen-Poiseuille liquid flow through a cylinder. The radius of the cylinder is modeled to vary with the amount of overlap between the contacting particles, hence with the amount of compressive forces.
\[ r = r_o - C \cdot U^n \]  

(2.11)

In the equation above, \( r_o \) (which in our case is a fraction of the average radii of the contacting particles) is the term which accounts for the background permeability; \( C \) is proportionality constant (between 0 and 1 in our model) and \( U_\alpha \) is the overlap distance at the contact between the two contacting particles. The parameter \( r_o \) is important and is in principle derivable from a calculation of the radius of the equivalent cylinder with the same flow conductivity as the space between two spherical particles in a 3-D geometry. However, in real rocks, the constituent sand particles are rarely nicely shaped spheres so in practice this is a tunable input parameter. As will be shown, permeability is very sensitive of the magnitude of \( r_o \).

The parameter \( C \) is a way to quantify the change in the conductivity of conduit between two pores when there is deformation. The flow through a pore throat is given by:

\[ q = \frac{\pi}{8\mu} r^4 \frac{\Delta P}{R_1 + R_2}, \]  

(2.12)

where \( r \) is the pore throat radius as defined above in Equation 2.31, \( \mu \) is the fluid’s viscosity, \( \Delta P \) is the pore pressure difference between the two connected pores, and \( R_1 \) and \( R_2 \) are the radii of the particles in contact.

The pressure response in a pore after a time step \( \Delta t \), due to the fluid flow and mechanical pore volume change, is given by:
\[ \Delta P_r = \frac{K_f}{V_p} (q \Delta t), \]  

(2.13)

in which \( K_f \) is the fluid’s bulk modulus, and \( q \) is the flow rate. For numerical stability the pressure change due to flow rate should be smaller than the initial pressure difference that causes the flow rate, \( \Delta P_r \leq \Delta P \). Hence the minimum fluid flow time step is given as

\[ \Delta t \leq \frac{8\mu(R_1 + R_2)V_p}{\pi K_f r^4}. \]  

(2.14)

The pore fluid pressure exerts a force \( F_i \) on each of its surrounding particles which in our model is approximated as

\[ F_i = P \cdot s \cdot n_i, \]  

(2.15)

where \( n_i \) is the unit normal vector of the line joining the two contact points on the particle, \( s \) is the length of that line and \( P \) is the pore pressure, as seen in the Figure 2.6.
The coupling between the mechanics and the fluid flow of the system allows the deformation that changes distances between the particles in contact to modify the conductivity of the pore throats. Strains induced by stresses and slipping and motion of particles makes old contacts vanish and new contacts formed, which in turn also changes the pore network of the system on which the transport properties of the sample are dependent. Fluid pressure applies forces to the individual particles surrounding the pore, contributing to the effective internal stress of the sample. It is possible therefore to conduct fluid flow experiments on samples brought into different stress-strain conditions by mechanical tests, and see how the fluid flow permeability depends on these conditions.
3 Mechanical Test Simulations

3.1 Sample Preparation

The sample consists of a dense packing of circular particles which are bonded by parallel bonds at their contact points in the case of cemented material, and unbonded for the case of uncemented. Particles radii are chosen from a linear distribution (Figure 3.1) and are generated in random locations within a space confined by walls (Figure 3.2). The particle radius distribution used in our simulations is (0.4-0.6 mm).

Following generation, ball radii are increased by a factor to achieve the desired 2-D porosity. After the radius increase, the samples are allowed to move and reposition without friction and bonding until the maximum average unbalanced force between particles becomes lower than 1% of the average contact forces between them. Figure 3.4 illustrates the particles and the compressive contact forces between them at this stage of sample generation. This step serves the purpose of eliminating locked in forces and stresses which would be unphysical and creating an isotropic stress state on the scale of several particles. If the magnitude of this isotropic stress is too large compared to the stresses the sample is supposed to experience under natural conditions, then the porosity is increased. If it is too low, the porosity is decreased. The porosity of unbonded samples is the lowest porosity for which the value of isotropic stress is negligible (in the order of kPa). In the case of weakly bonded sample the porosity is 0.15, this value of porosity gives a value of about 3 MPa for the isotropic stress.
After this step is achieved, the floating particles are eliminated. Floating particles are particles which are in contact with less than 2 other neighboring particles and hence do not contribute to the interior stress state of the sample. When we model the cemented sandstones the next step is the creation of bonds and activation of friction between the particles. After this step the walls on the weakly bonded sample are removed and the sample is allowed to expand and relax. The force chain network changes during this step as illustrated in Figure 3.5. If the sample disintegrates by bond breakage during this relaxation period after the wall removal, it means that the bonds’ strength and size are not high enough and their magnitude is increased. The other criteria for the strength of the parallel bonds are the unconfined compressive and triaxial tests done on the samples.

Because of the random size and location the particles are generated, no two samples created with the same micro mechanical parameters would be identically the same and have the same macroscopic properties. However for a sufficiently high number of particles, the differences in macroscopic behavior become negligible. About 8,500 particles are generated in our simulated samples and the sample size is 4x4 cm.
Figure 3.1: Particle radius probability distribution.

Figure 3.2: Balls and compression forces between them after the balls have moved and unbalanced forces are sufficiently low. This is the stage when the balls are bonded and friction is activated.
Our approach in modeling the cemented samples is an attempt to simulate the life cycle of a real sedimentary clastic rock, namely the stages of deposition, compaction and cementation as described in Jin et al. (2003) and McBride (1989). The bonded sample’s particles have the same micromechanical properties which are fitted to experimental results done on uncemented sands (deposition). Then the porosity is decreased by increasing the particles radii by a factor, during which phase the internal isotropic stress increases (compaction). In the case of unbonded samples, the porosity is decided as the lowest porosity which gives rise to a very small isotropic stress (on the order of kPa). In the case of weakly bonded samples, the porosity is decided as the value which gives rise to an isotropic stress in the order of 3 MPa. Then the particles of the weakly bonded samples are
bonded by parallel bonds with mechanical properties similar to those of the particles (cementation).

3.2 Choosing the micromechanical parameters

The micromechanical parameters required for a model using the DEM method of PFC are relatively few. Quantifying the constituent grains requires three parameters: the Young’s modulus of the particles, \( E \), the normal to shear stiffness of the particles, \( \frac{k_n}{k_s} \), and the interparticle friction coefficient, \( \mu \). The density of the grains plays no role in the mechanical behavior of the sample because only the static (equilibrium) solution of the equations of motion is found (Itasca, 2001). Characterizing the bonds requires five parameters: \( E, \frac{k_n}{k_s}, \sigma_c, \tau_c \) and \( \lambda \). \( E \) is the Young’s modulus of the bond, \( \frac{k_n}{k_s} \) is the normal/shear stiffness ratio associated with the bond, \( \sigma_c \) and \( \tau_c \) are the tensile and shear strength of the bond in units of stress, and \( \lambda \) is the bond size multiplier. The bond size is related to the radius of the smallest particle of the pair with Equation 3.1:

\[
\bar{R} = \lambda \cdot R_i
\]
The normal stiffness of the particle \( k_n \) may be found in relationship to \( E \) using the equivalent beam theory of the equivalent continuum material of the grain-cement-grain or grain-grain system. (Potyondy and Cundall 2004).

If \( t \) is assigned to be the unit thickness of the cylinders in the PFC-2D model and \( L \) the length of the beam in the Equations 3.2 and 3.3:

\[
\frac{k_n}{2} = \frac{L \cdot t \cdot E}{L} \Rightarrow k_n = 2E .
\]  

Similarly, the stiffness of the cement can be written as:

\[
\bar{k}_n \cdot A = \frac{A \cdot \bar{E}}{R_A + R_B} \Rightarrow \bar{k}_n = \frac{\bar{E}}{R_A + R_B},
\]

where \( A \) is the cross sectional area of the beam.
The stiffness of the particles themselves is independent of the particle radii. However the bond elastic stiffness (rather stiffness density) is dependent on the particle radii and hence has to be scaled accordingly.

The $\frac{k_n}{k_s}$ ratio is related to Poisson’s ratio; for a realistic Poisson’s ratio of the material this ratio has to be bigger than 1 (Potyondy and Cundall, 2004). After assigning a value to this ratio the shear stiffness of the particle and the bond can then estimated by:

$$k_s = \frac{k_n}{k_n/\bar{k}_s},$$

and

$$\bar{k}_s = \frac{k_n}{k_n/\bar{k}_s}$$ (3.4)

The particle’s Young Modulus $E$ could ideally be estimated from the mechanical properties of the minerals that constitute the grains. The mineralogy of many rocks and Young moduli of many minerals are available. In practice, because of the presence of clay at the grain boundaries it is difficult to assign an average value for the Young modulus $E$ to the grains and fitting to experimental data is necessary. The bond size multiplier $\bar{\lambda}$ is close to 1 for a strongly bonded material. The bond strengths $\bar{\sigma}_c$ and $\bar{\tau}_c$ can be estimated by knowing the mineralogy of the rock and values of tensile strengths.
But for complex pore geometries and multi-mineral case calibration is necessary. Experimental results of triaxial Young’s moduli and peak strengths for uncemented sands by Yaich (2008) are used to fit for the particle Young’s modulus and for the friction coefficient.

The parameters which control the macroscopic mechanical behavior of an unbonded sample are the particles’ Young’s modulus, coefficient of friction and the two dimensional porosity. The value for the porosity is decided on the basis of the closest random packing of the particles which gives rise to a negligible isotropic stress after the particles are generated, repositioned and the forces have balanced. The lowest value of porosity where this is achieved is 18% (Figure 3.5) and it is this value for the initial porosity we have chosen for the unbonded sample. The particles’ Young modulus controls the macroscopic Young’s modulus of the sample during a triaxial test. It also controls up to an extent the maximum stress before ductile failure. The friction coefficient, on the other hand, is the main factor which controls the peak stress under a triaxial test for unbonded samples.

Figure 3.6 shows differential stress versus vertical strain during triaxial tests of unbonded samples with different particle Young’s moduli. The horizontal $S_{xx}$ and vertical stresses $S_{yy}$ are defined as the measured force on the walls divided by the area of the walls (their length times the unit thickness). The horizontal, vertical and volumetric strain, $E_{xx}$, $E_{yy}$ and $E_{vol}$, are defined as negative for expansion and positive for contraction as in Equation 3.6, and the differential stress $S_{dev}$ as in Equation 3.7.
\[ E_{xx} = - \frac{\Delta x}{\text{Width}} \]
\[ E_{yy} = - \frac{\Delta y}{\text{Height}} \]  \hspace{1cm} (3.6)
\[ E_{\text{vol}} = E_{xx} + E_{yy} \]
\[ S_{\text{dev}} = S_{yy} - S_{xx} \]  \hspace{1cm} (3.7)

A range of 0.12-0.24 GPa for the value of particle Young’s modulus was tested. The other micro parameters were kept constant and are those of Table 3.2. The triaxial test was performed under a 0.35 MPa confining stress. Increasing the particle stiffness increases the macroscopic Young’s modulus of the sample. It also increases the peak stress. The dependency of the macroscopic Young’s modulus to the particle Young’s modulus is linear, as shown in Figure 3.7. For the variation range of 0.12-0.24 GPa in particle Young’s modulus, a variation of 58-90 MPa in macroscopic sample’s Young’s modulus is observed. These values are comparable to the values measured experimentally by Yaich (2008).

Figure 3.8 shows differential stress versus vertical strain during triaxial tests of 0.35 MPa confining pressure of unbonded samples with different friction coefficients. All the other micromechanical parameters were kept constant, and are those of Table 3.2. A range of friction coefficients of 0.4-1.2 was tested. The friction coefficient has no effect of the macroscopic Young’s modulus of the sample, but it increases the triaxial peak differential stress strength of the sample. For the range of friction coefficients tested, a range of 0.58-1.32 MPa peak differential stress was observed. The dependence of the
peak stress on the friction coefficient for the triaxial tests of Figure 3.6 is shown in Figure 3.9. The dependence is linear for reasonable (<1) values for the friction coefficient.

The effect of bond strength in bonded samples is shown in Figures 3.10 and 3.11. Figure 3.10 shows compressive stress versus vertical strain during unconfined compressive tests of bonded samples with different bond strengths. A range of 10-35 MPa for the bond strength was tested. All the other parameters are kept constant and are those of Table 3.1, with the exception of bond radius multiplier which is 1.0. As expected the bond strength increases the unconfined strength of the bonded samples. A range of 19-63 MPa strength was observed for the range of bond strengths tested. Figure 3.11 shows that unconfined strength of the bonded samples varies linearly with bond strength if all the other micro parameters are kept constant. As expected, bond strength does not affect the macroscopic Young’s modulus.

Figures 3.12 and 3.13 show the bond size effect on the unconfined compressive strength of bonded samples. A range of 0.5-1.0 for the bond size multiplier was tested with all the other microscopic parameters kept constant, except for the bond strength which is assigned a value of 30 MPa. The other parameters are those of Table 3.2. Figure 3.12 shows the compressive stress versus vertical strain during unconfined compressive tests of bonded samples with different bond size multiplier Lambda. The bonded samples’ unconfined strength increases with bond size multiplier; however this dependence is not simply linear, as seen in Figure 3.13. This dependence on the bond size is qualitatively similar to the field data of samples with different degrees of effective quartz overgrowth from the Unayzah and Jauf formations (Al Tahini et al., 2006). A
variation in the UCS from 25 to 200 MPa is observed in cores with similar porosities but with a different amount of cementation/quartz overgrowth.

The normal to shear elastic stiffness ratio of the particles, $\frac{k_n}{k_s}$, affects the macroscopic Poisson’s ratio of the sample. The Poisson’s ratio increases with increasing stiffness ratio. It is assigned a value of 5 in all our simulations.

The parallel bonds elastic Young’s modulus $\bar{E}$ is assigned to be 0.75E on the assumption that the mechanical properties of the cement are similar to those of the constituent grains in sandstones (McBride, 1989). The stiffness ratio $\frac{k_n}{k_s}$, on the other hand is assigned a value of unity.

Our criteria for the properties of a weakly cemented rock are the unconfined compressive strength and Young’s moduli of the rocks. UCS of the weakly bonded sample is about 15.1 MPa, and the unconfined elastic Young’s modulus is 1.02 GPa. This is within the boundaries of the definition of poorly cemented sands by Al Tahini et al., 2006; Abbas et al., 2002; Nikraz and Evans, 1999; Dautriat et al., 2007; Nicholson et al., 1998 and Ruistuen et al., 1996. In these works rocks with UCS lower than 30 MPa and Young’s moduli in the range of 0.5 to 5 GPa have been described as poorly cemented sands and are associated with compaction and subsidence, sand production and productivity reduction due to decreases in permeability. The micro parameters of a weakly bonded rock used in our simulations are those of Table 3.2. The weakly bonded sample with which we simulate the mechanical and flow properties of the poorly
cemented sands has a 2 dimensional porosity of 0.15. This value of porosity causes an isotropic stress of 3.0 MPa (Figure 3.5) at the end of the sample generation, before the sample is bonded (Section 3.1). It is our assumption that in shallow or overpressured reservoir conditions poorly cemented sands exist at this order of effective stresses (Dautriat 2007 and Abbas 2002). It has a bond size multiplier of 0.5 and bond strength of 15 MPa. The particles’ elastic Young modulus and friction coefficient are fitted according to the triaxial tests performed by Yaich 2008 and are assigned a value of 0.21 GPa and 0.8 respectively.

![Isotropic stress changing with 2-D porosity](image)

*Figure 3.5: Isotropic stress at the end of sample generation procedure of the unbonded sample as a function of initial 2-D porosity.*
Figure 3.6: Triaxial test of unbonded samples with different particle Young’s moduli. Confining stress is 0.35 MPa for all tests.

Figure 3.7: Unbonded sample's macroscopic Young's modulus' dependence on the particles' Young modulus.
Figure 3.8: Triaxial tests of unbonded samples with different friction coefficient. Confining stress is 0.35 MPa for all tests.

Figure 3.9: Dependence of triaxial differential strength of unbonded samples on the value of friction coefficient.
Figure 3.10: Unconfined compressive tests of bonded samples with different bond strengths. 2-D porosity is 0.15 and the bond size multiplier is 1.0.

Figure 3.11: Unconfined strength of bonded samples with different bond strength. 2-D porosity is 0.15 and the bond size multiplier is 1.0.
Figure 3.12: Unconfined strength of bonded samples with different bond strength. 2-D porosity is 0.15 and the bond size multiplier is 1.0.

Figure 3.13: Dependence of UCS on the bond size multiplier Lambda.
Table 3.1: Micromechanical and test parameters of the unbonded samples.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Young’s Modulus $E$</td>
<td>0.21 GPa</td>
</tr>
<tr>
<td>$R_{\text{min}}$</td>
<td>0.4 mm</td>
</tr>
<tr>
<td>$R_{\text{max}}$</td>
<td>0.6 mm</td>
</tr>
<tr>
<td>Sample dimensions</td>
<td>4x4 cm</td>
</tr>
<tr>
<td>2-D porosity</td>
<td>18%</td>
</tr>
<tr>
<td>Normal/Shear Stiffness Ratio $k_n/k_s$</td>
<td>5</td>
</tr>
<tr>
<td>Friction Coefficient $\mu$</td>
<td>0.8</td>
</tr>
<tr>
<td>Axial Strain Rate $E_s^{-1}$</td>
<td>$1.0E-6 \cdot \frac{1}{s}$</td>
</tr>
</tbody>
</table>
Table 3.2: Micromechanical and test parameters of the weakly bonded samples.

<table>
<thead>
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<th>Parameter</th>
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</tr>
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<td>5</td>
</tr>
<tr>
<td>Friction Coefficient $\mu$</td>
<td>0.8</td>
</tr>
<tr>
<td>Bond Young’s Modulus $\bar{E}$</td>
<td>0.75$E$</td>
</tr>
<tr>
<td>Bond Multiplier $\lambda$</td>
<td>1.0</td>
</tr>
<tr>
<td>Bond normal/shear Stiffness Ratio $\frac{k_n}{k_s}$</td>
<td>1.0</td>
</tr>
<tr>
<td>Bond Tensile Strength $\sigma_c$</td>
<td>15.0 MPa</td>
</tr>
<tr>
<td>Bond Shear Strength $\tau_c$</td>
<td>15.0 MPa</td>
</tr>
<tr>
<td>Strain Rate</td>
<td>$1.0E - 6 \cdot \frac{1}{s}$</td>
</tr>
</tbody>
</table>
3.3 Hydrostatic Compression Tests

Hydrostatic compression tests are conducted on both bonded and unbonded samples by having the confining walls come towards each other at equal constant speed, such that the stresses in both horizontal and vertical directions are the same. A plot of hydrostatic stress versus volumetric strain for an unbonded sample is shown in Figure 3.14. The sample is compressed up to a value of 4.6 % volumetric strain (loading), after which the walls velocities are reversed (unloading). A maximum hydrostatic stress value of 5.4 MPa is achieved at 4.6 % volumetric strain value. The stress strain curve is linear and the sample’s bulk modulus which is the slope of the line is measured to be 116 MPa. The stress strain curve continues on the same line back during the expansion stage of the test, no hysteresis is observed.

Figure 3.15 shows a plot of hydrostatic stress versus volumetric strain for a weakly bonded sample. The hydrostatic stress increases linearly with volumetric strain up to a value of 2.7% of strain and 17 MPa stress. The elastic bulk modulus value, which is the slope of the line up to that point, is 0.67 GPa. After the 2.7 % value of strain the slope of the stress-strain curve decreases. The stress value at this point is the maximum hydrostatic stress the weakly bonded sample can withhold without having the bonds broken. The slope of the stress-strain curve is much lower after this point; with a bulk modulus of about 100 MPa; a value comparable to that of unbonded sample. Figure 3.16 shows the evolution of the broken bonds with volumetric strain rate at equal intervals, starting from 2.5% strain value to the end of compression stage of the test. The first bonds break at 2.5% volumetric
strain and the number of broken bonds increases rapidly with volumetric strain. The broken bonds are not generated randomly throughout the sample; they tend to group together and the new broken bonds tend to happen in the vicinity of the already broken ones. However there is no preferred direction along which the bonds break.

During the expansion stage of the test, hysteresis in the stress curve is observed; the stress values are lower than the values at the same strain values during compression. This is because the mechanical state of the system has changed irreversibly due to the broken bonds. Teufel et al. (1996) reports a bulk modulus between 2-4 GPa for weakly cemented Oseberg sandstones. They also report a dependence of bulk moduls on the effective stress of the sample which is also the case in our simulations. For the range of hydrostatic stresses applied to the weakly bonded sample, the elastic bulk modulus decreases after a critical stress value (17 MPa). Weak limestone samples show the same kind of pore collapse behavior our simulations during uniaxial strain compression experiments (Soares et al. 2002). Zaman et al. (1993) and Saidi et al. (2005) report the same behavior of weakly cemented sandstones and chalk, where pore collapse happens at critical hydrostatic pressure after an elastic dependence between stress and volumetric strain.
Figure 3.14: Hydrostatic stress versus volumetric strain during hydrostatic compression of unbonded sample.

Figure 3.15: Hydrostatic stress versus volumetric strain during hydrostatic compression test of weakly bonded sample.
3.4 Unconfined Compressive Tests on Weakly Bonded Samples

Unconfined compressive tests are realized after the sample generation procedure by having the two vertical walls (side) removed from the system and the horizontal walls (top and bottom) come towards each with a constant speed and compressing the sample. The horizontal $S_{xx}$ and vertical $S_{yy}$ stresses are defined as the measured force on the walls divided by the area of the walls which is their length times the unit thickness. The
micromechanical and test parameters used to generate the results shown are given in Table 3.2.

The weakly bonded sample fails in a brittle way at 1.8% axial strain at a compressive stress value of 15.4 MPa (Figure 3.15), after which the compressive stress’s value decreases. The stress-strain curve may be divided into 3 regimes; the elastic regime (from 0 to 1.8% strain), the failing regime (from 1.8 to around 4 %), and the sliding regime (4% to maximum strain value). The elastic regime is the regime in which stress increases linearly with strain and the bonds are still intact. The failing regime is the regime in which the bonds break along a preferred direction. The stress decreases during the failing regime. The sliding regime is the regime in which the broken and separated blocks of the sample slide past each other and the only resistance is friction. Stress remains low but relatively constant during this regime.

The evolution of the pattern of the broken bonds during the unconfined compressive test is shown in Figure 3.16. Bonds start to break at around 1.5% axial strain value. Figure 3.16 shows snapshots of broken bonds due to tension (blue) and due to shear stresses (red) at equal strain interval starting from 1.5% till the end of the test at 6.8%. Bonds broken due to tension are initially scattered without a pattern through the sample, as seen in the first 2 snapshots of the figure. However they start to group, as the axial strain increases, in a preferred orientation, diagonally to the sample. The majority of the broken bonds are tension induced, however at higher strain value, shear induced broken bonds are generated as well. Shear induced broken bonds seem to not follow the preferred orientation
pattern of the tension induced broken bonds. Instead they are scattered randomly throughout the sample, with a higher concentration close to the top and bottom sides of the sample. The formation of the failed bands with a diagonal orientation is similar to the observation on the unconfined compressive tests done on synthetic weakly cemented sands by Nikraz and Evans (1999) and experimental results conducted on consolidated sandstones by Maurer (1965).

Unconfined compressive tests were run on samples with different porosities to see the effect of porosity on the unconfined strength and Young’s moduli of the samples. The other micro-mechanical and test parameters were kept the same and are those of Table 3.2, with the exception of bond strength and bond size multiplier, which are assigned values of 30 MPa and 1.0 respectively. The results of the variation of unconfined compressive strength with porosity are shown in Figure 3.19. A range of 0.10 to 0.185 2-D porosity was tried. Unconfined compressive strength decrease with increasing porosity; a variation of unconfined strengths of 70 to 18 MPa is observed. Young’s modulus also decreases with increasing porosity as seen in Figure 3.20. For the range of 2-D porosities tested a variation of 1.85 to 0.75 GPa in samples’ macroscopic Young’s modulus is observed. These results are qualitatively similar to the data from Unayzah and Jauf cores (Al-Tahini, 2006), where unconfined compressive strength of the cores are reported to depend on their porosity. A range of 10 to 80 MPa in the UCS is reported for a range of porosities from 0.3 to 0.04. Eldmann (1998) also reports a relationship between UCS and porosities of cemented
sandstone from North Sea various fields; a variation from 10 to 180 MPa is observed for a range of variation from 0.4 to 0.05 in porosity.

Figure 3.17: Compressive stress versus strain in an unconfined compressive stress of a weakly bonded sample.
Figure 3.18: Broken bond configuration on the weakly bonded sample at different equally spaced axial strain values, starting from 1.5% strain till the end of the test at 6.8% strain value. Blue is tension induced broken bonds and red is shear induced broken bonds.
Figure 3.19: Unconfined compressive strength versus 2-D porosity for bonded samples.

Figure 3.20: Macroscopic Young's modulus versus porosity for bonded samples during unconfined compressive tests.
3.5 Triaxial Tests

Our samples are all in 2-D hence truly the tests we run are biaxial tests in plane strain conditions (Potyondy and Cundall, 2004). However it is the mechanical properties that one finds out from a true three dimensional triaxial test that we are interested in simulating. For this reason, terms such as horizontal and radial, vertical and axial, as well as area and volume will be used interchangeably. In our simulations, a triaxial test is a test in which axial shortening increases (in the y direction) while the horizontal stress, \( S_{xx} \) is kept constant by means of a servo mechanism. The servo mechanism routine works following these steps (Itasca 2001):

1. Initially a value for the horizontal and/or vertical stress is specified.

2. The contact forces and stresses on each wall are measured.

3. If the measured stress is higher than the specified stress the wall moves out of the sample with a speed proportional to the difference. If the measured stress is lower than the desired stress value the wall moves into the sample with a speed proportional to the difference between the measured and specified stress. The speed \( v_w \) is determined by (Cundall, 1988):

\[
v_w = \frac{\alpha A}{k_n N_c \Delta t} \cdot \Delta \sigma,
\]

(3.5)
in which $\alpha$ is a relaxation factor necessary for numerical stability, $A$ is the area of the wall (length times unit thickness), $k_n^w$ is the elastic stiffness of the wall (set to be equal to the ball stiffness), $N_c$ is the number of ball contacts with the wall which is updated for each calculation step, $\Delta t$ is the calculation time step and $\Delta \sigma$ is the difference between the measured and the desired stress. In our case $\alpha = 0.5$.

4. The forces within the sample are allowed to balance and the new stress on the wall is measured.

5. If the stress difference, $\Delta \sigma$, is not within a tolerance value of 1%, steps 2 through 4 are repeated again.

Before the triaxial test is started, the sample is brought under a determined isotropic stress state. After this state has been achieved, the horizontal walls (top and bottom) move towards each other with a constant speed, while the vertical walls (side) are acting under the servo mechanism to keep the horizontal stress constant. This is the loading part of the test. After achieving a high enough vertical strain value, the sample is then unloaded by reversing the velocity of the moving horizontal walls; this is the unloading stage of the test.

We also ran numerical tests in which the confining (lateral) stress was decreased after the application of a moderately high isotropic stress, which we call a radial expansion test. Similarly to the compressive triaxial tests, the behavior of the material when the walls start coming together after an expansion stage is studied as well (compaction).
3.5.1 Compressive Triaxial Tests

We ran triaxial tests on the two types of samples, unbonded and weakly bonded. The triaxial test results of the unbonded sample are shown in Figure 3.21. The horizontal confining stress is 0.35 MPa. The test for the unbonded samples was conducted until 6.4% axial strain value. After the initially elastic compressive region, the unbonded sample fails in a strain softening ductile fashion. The sample’s elastic Young’s modulus is measured to be $E=87$ MPa. The elastic regime of the stress strain curve ends at about 1% strain value, after which the sample goes into ductile failure. Volumetric strain increases during the elastic compressive region of the loading stage. It starts to decrease and take negative values during the ductile failure region which indicates dilatation. Horizontal strain, on the other hand, remains zero up to about 0.5 % axial strain value, after which it decreases (the sample expands horizontally). The differential stress takes negative values during the unloading stage of the triaxial test. The unloading stage of the triaxial test of the unbonded sample may still be divided into two regimes, the abrupt decrease in differential stress initially and the relatively constant, low value stress regime. There is path hysteresis in all three measured properties of the sample; differential stress, horizontal and volumetric strain. During the unloading stage of the test, neither of these properties follows the path of the loading stage.

Triaxial test results of a weakly bonded sample are shown in Figure 3.22. The horizontal confining stress is 0.35 MPa. The maximum axial strain value tested was 3.4%. Brittle failure occurs at about 1.9% of axial strain and at a maximum differential stress
value of 15.6 MPa, after which the vertical stress drops abruptly. The sample’s elastic Young’s modulus is measured to be 1.12 GPa. The volumetric strain increases until the failure point, after which it decreases and takes negative values. The horizontal strain on the other hand remains zero up until the failure point, after which it takes negative values (the sample expands horizontally) Similar to the case of unconfined compressive test the loading stress-strain curve may be divided into 2 regimes; the elastic regime (from 0 to 1.9% strain) and the failing regime (from 1.9 to 3.4%). The elastic regime is the regime in which stress increases linearly with strain and the bonds are still intact. Bonds break along a preferred direction, which is vertical or at a small angle to the vertical direction during the failing regime and the differential stress decreases. The friction-only sliding regime is not shown on the graph because we do not go to high enough strain values. The unloading phase of the triaxial test starts after the brittle failure, at 3.4% during which the differential stress decreases even further until it reaches the value zero at the end of the test. There is path hysteresis in all three measured properties of the sample; differential stress, horizontal and volumetric strain. During the unloading stage of the test, neither of these properties follows the path of the loading stage. This is because the sample’s mechanical properties have changed irreversibly because of brittle failure.
Figure 3.21: Differential stress (top), radial and volumetric strain (bottom) versus axial strain during a triaxial test on an unbonded sample. The confining stress is 0.35 MPa.
Figure 3.22: Differential stress (top), horizontal and volumetric strain (bottom) versus axial strain during a triaxial test on a weakly bonded sample. The confining stress is 0.35 MPa.
3.5.2 **Effect of Confining Pressure during Conventional Triaxial Test**

Triaxial tests of different confining stress were conducted on the same unbonded sample. The unbonded sample’s micromechanical parameters were those of Table 3.1. The range of confining stresses tried on the unbonded sample was from 0.2 MPa to 4.5 MPa. At higher confining stresses the unbonded sample’s peak differential stress increases, as well as the strain value where failure occurs (Figure 3.23). A variation from 1.1 to 8.9 MPa in the peak differential stress the unbonded sample endures is observed for the range of confining pressures tested. The sample’s macroscopic Young’s modulus during the elastic portion of the test and the general shape of the stress strain curve remain unaffected. Figure 3.24 shows a plot of the shear stress versus that of average stress at failure for the triaxial tests with different confining pressures on the unbonded sample. The dependence is linear with a correlation coefficient of almost unity for the range of confining stresses tested.

The effect on the confining stress value on triaxial test results is more pronounced on the bonded samples. Figures 3.25 shows triaxial test results with different confining pressures on the weakly bonded samples. A range of 0.5 to 8.0 MPa confining pressures is tested on the weakly bonded sample. Up to a threshold value, both the weakly and strongly bonded samples peak differential stress increases with confining pressure. However after that value, the failure mode of the bonded samples changes. The failing mode changes from strain-softening to strain-hardening. This threshold confining pressure value is about 4 MPa. The difference in the micromechanics of the system is shown in Figure 3.26, which
shows the pattern of broken bonds of a weakly bonded sample at the end of a triaxial test with a confining pressure of 0.35 MPa (left) and 6.0 MPa (right). For low confining pressure, broken bonds are localized and oriented in a preferred direction, whereas under high confining pressure, broken bonds are more randomly oriented. The majority of the broken bonds at low confining pressure are tension induced (blue) whereas in the case of high confining pressure, shear induced broken bonds are about the same number as the tension induced. The density and number of the broken bonds is also higher in the case of higher confining pressure triaxial tests. Tension induced broken bonds tend to orient in a preferred direction whereas the shear induced broken bonds occur throughout the sample without any preferred direction.

Figure 3.23: Differential stress versus axial strain during triaxial tests of different confining pressures of unbonded samples.
Figure 3.24: Shear stress versus average normal stress at failure during triaxial tests for unbonded samples.

Figure 3.25: Differential stress versus axial strain during triaxial tests of different confining pressures of weakly bonded samples.
3.6 Radial Expansion Failure Simulations:

Besides conventional triaxial test simulations, another type of failure mechanism in bonded and unbonded samples is simulated. The sample is initially brought into hydrostatic stress, then the side stress $S_{xx}$ is decreases gradually by making the vertical side walls move away from each other (expansion phase) with a constant speed. After achieving a certain horizontal strain value, the walls start coming back (compaction phase). The stress on the horizontal walls (top and bottom) is kept constant by means of the servo mechanism. The unbonded sample’s parameters are given in Table 3.1 and the weakly bonded parameters are given in Table 3.2. For the results shown here the initial hydrostatic stress is 1.5 MPa for the unbonded sample and 15 MPa for the weakly bonded sample

Figure 3.27 shows the stresses and volumetric and vertical strains of an unbonded sample during a radial expansion test. The side walls move apart (expansion) up to -1.97%
horizontal strain value after which they come towards each other (compaction) up to -1.0% horizontal strain value. Horizontal stress decreases linearly with horizontal strain up until 0.4% strain value after which it remains constant at 0.6 MPa for the duration of the expansion stage of the test. 0.4% is also the value of the strain at which the slope of the vertical and volumetric strains changes. The slope of the linear decrease in stress with horizontal strain is 160 MPa. Volumetric strain decreases up to -0.8% and vertical strain increases up to a value of 1.3 % during the expansion stage of the test. Horizontal stress increases during the compaction stage and increases up to a 1.2 MPa value at 1.0 % horizontal strain. Volumetric strain increases and the vertical strain decreases during the compaction stage of the test. As with the case of triaxial tests, there is hysteresis in all these three quantities; none of them follows the previous expansion path. This is because the sample has failed and its mechanical properties have changed in an irreversible way.

Stresses and volumetric and vertical strains of a weakly bonded sample during a radial expansion test are shown in Figure 3.26. The side walls move apart (expansion) up to a 1.3% horizontal strain value after which they come towards each other (compaction) up to 0.65% horizontal strain value. Horizontal stress decreases linearly with horizontal strain till about 1% horizontal strain, after which point the value of horizontal stress remains constant. The slope of the linear decrease in stress is very close to the Young’s modulus of the sample, 1.01 GPa. Horizontal stress increases during the compaction stage and increases up to a 1.2 MPa value at 1.0 % horizontal strain. Volumetric strain initially decreases with horizontal strain till 0.8% strain value, after which it increases. 0.8% is also
the value of horizontal strain at which the rate of increase in vertical strain increases. Volumetric strain increases and the vertical strain decreases during the compaction stage of the test. Similarly to the unbonded sample radial expansion test, there is path hysteresis in all these three quantities; they do not follow the previous expansion path. This is because the sample has failed, bonds are broken and the mechanical properties have changed irreversibly.
Figure 3.27: Vertical and horizontal stresses, volumetric and horizontal strain versus radial (horizontal) strain during a radial expansion test on an unbonded sample. The initial hydrostatic stress is 1.5 MPa.
Figure 3.28: Vertical and horizontal stresses, volumetric and horizontal strain versus radial (horizontal) strain during a radial expansion test on a weakly bonded sample. The initial hydrostatic stress is 15.0 MPa.
4 Permeability Variation Simulations

4.1 Procedure

The micromechanical parameters used in the mechanical experiments are used in the samples used for the fluid flow experiments as well, because the transport properties are also dependent on the mechanical properties of the materials. The procedure for the fluid flow experiments goes through the same sample generation as described in section 3.2.

For the permeability variation during mechanical tests, the walls’ velocities are zeroed at the desired strain value. After this, the domain building (pores and pore structure building) routine is applied on the sample. After the pore structure has been built, every pore on the structure is assigned a pore pressure depending on its position on the sample, such that a linear pressure profile is generated in the direction of the desired fluid flow. This is done to save time; the net result, which is the measurement of the flow rate and permeability, is the same as invading fluid from one end of the sample and waiting until the Darcy regime has been established numerically. The maximum pressure on any pore is 1000 Pa, negligible compared to the interior stresses on the sample. Hence the effect of fluid pressure and drag on the particles is negligible.
Figure 4.1: Pressure profile on x-direction permeability measurement simulations.

Figure 4.2: Detail on how the flow rate through a line (black) along the sample is measured. Flow rates through all the pore throats which cut the black line (surrounded by the blue rectangles) are added for the calculation of permeability.
When the linear pressure profile is generated, the flow rate is measured at different lengths along the sample. The flow rate at a certain length along the sample is calculated as the sum of flow rates through all the pore throats that connect pores which lie on different sides of the line that marks that length. Figures 4.1 and 4.2 give an illustration of the method. Ideally for an incompressible fluid flow through porous media the flow rates at any length on the sample should be the same. However because the sample does not have an infinite number of pores and pore throats there is some difference because of the way the flow rate is numerically calculated. Flow rates at any length along the sample are within 15% of each other. The flow rate we use for the permeability estimation is the average of the flow rates measured along three lines along the sample, a line through the quarter length of the sample, a line through the middle and a line that passes through the three quarter length of the sample. Permeability is then estimated by the formula:

$$K = \frac{Q \cdot \mu}{A \cdot \Delta P / L}$$  \hspace{1cm} (4.1)$$

where $K$ is the permeability, $Q$ is the average flow rate, and $\mu$ is the fluid viscosity.

The coupling between fluid flow and mechanics of the system in this method happens before the fluid flow simulation. The step where the coupling happens is the domain building step. Samples at different stress states will have different intraparticle forces and overlaps between them. Also, because the particles are allowed to move during deformation, the domain structure will be different at different stress-strain states of the sample.
4.2 Choosing the fluid flow micro properties

The mechanical input parameters for the particles and bonds are the same as the ones used in the mechanical experiments. The mechanical properties of the materials do not vary with the size of the particles and sample because the relevant parameters are scaled appropriately. However, permeability is scale dependent and the parameters need to be adjusted for the grain size. The two adjustable parameters in our model are the coefficient $C_1$ and the coefficient $C_2$ in Equations 4.2 and 4.3. $C_1$ determines the magnitude of the equivalent cylinder with the same fluid conductivity as the contact between two particles. $C_2$ determines by how much the equivalent cylinder’s radius decreases when the particles overlap with an overlap distance of $U^n$:

$$r = r_o - C_2 U,$$

$$r_o = C_1 \cdot R_B.$$  \hspace{1cm} (4.2) \hspace{1cm} (4.3)

$R_B$ is the radius of the smallest ball of the contact, $U$ is the overlap amount and the parameter $r_o$ is a fraction $C_1$ of the radius of the smallest ball that forms the contact.

Fluid flow experiments of unbonded samples under 1 MPa hydrostatic stress were simulated for unbonded samples with different $C_1$ parameters. The range of values tested was 0.05 to 0.55 and the value of the parameter $C_2$ was 1.0 in all the simulations. All the mechanical parameters’ values are those of Table 3.1. As seen in Figure 4.3, permeability is strongly dependent on the magnitude of $C_1$. The permeability value is 6 orders of
magnitude higher for the maximum value of $C_1$ (0.55) compared to the minimum value tested (0.05).

Fluid flow experiments were also simulated for unbonded samples under 5 MPa hydrostatic stress conditions with different $C_2$ parameters. The value of the $C_1$ parameter was set to 0.15 and all the other micromechanical parameters’ values are those of Table 3.2. Figure 4.4 shows that permeability decreases with increasing $C_2$ value. The dependency of permeability with $C_2$ increases as the hydrostatic stress increases. According to these results the values of the parameters $C_1$ and $C_2$ are decided for each kind of sample we ran permeability variation with. $C_2$ is assigned a value of 1.0 for each kind of sample, $C_1$ is assigned a value of 0.45 for the unbonded sample, such that the permeability at low stresses is around 100 Darcy (Yaich, 2008), a value of 0.20 for weakly bonded samples, such that the permeability of the sample is in the order of 5-10 Darcy at low stresses (Ruistuen et al., 1996; Schutjens et al., 2004). Table 4.1 shows these parameters.
Figure 4.3: Permeability Variation with the parameter C1. The gap multiplier parameter C2 is set to 1.0. The hydrostatic stress is 1 MPa.

Figure 4.4: Effect of gap multiplier C2 on the permeability. C1 is set to 0.15. The hydrostatic stress is 5 MPa.
Table 4.1: Mechanical and fluid flow parameters of the samples.

<table>
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<tr>
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<th>Unbonded</th>
<th>Weakly Bonded</th>
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<tr>
<td>Mechanical and Test Parameters</td>
<td>Table 3.1</td>
<td>Table 3.2</td>
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<tr>
<td>$C_1$</td>
<td>0.45</td>
<td>0.20</td>
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<tr>
<td>$C_2$</td>
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4.3 Permeability variation with initial porosity

Permeability simulations under 1 MPa hydrostatic stresses for bonded samples of different initial porosities were conducted. The range of 2-D porosities tested for the bonded sample is 0.10 to 0.18. The micromechanical parameters are those of Table 3.2 with the exception of bond strength and size, which are assigned values of 30 MPa and 1.0 respectively. The values of $C_1$ and $C_2$ are 0.15 and 1.0, respectively. There is a clear increasing permeability versus porosity trend in the case of bonded samples as seen in Figure 4.5. For the range of 2-D porosities tested a variation of 0.65 to 3.4 Darcy in permeability is observed.

There is a great body of literature regarding the relationship between porosity and permeability for different kinds of rocks. Our results do not agree with the Carman-Kozeny formula for permeability if we assume a constant tortuosity value for different porosities. The Carman-Kozeny formula would result in a greater variation of permeability with
porosity. For the range of porosities tested a change of at least one order of magnitude would be expected. Davies and Davies (2001) report permeability changing with porosity for un cemented sands from the Gulf of Mexico and Southern California formations. The permeability-porosity relationship depends on the rock type and there is a better correlation between the two quantities for better sorted sands. A good correlation of permeability and porosity is observed in a well sorted unconsolidated sand from the Gulf of Mexico with an average grain size of 120 microns. A range in permeability of 0.4 to 1 Darcy is observed for a range of porosities from 0.27 to 0.4. However their results show that permeability is more dependent on the grain size distribution than porosity.

![Permeability vs Porosity](image)

**Figure 4.5:** Permeability versus initial bonded sample porosity. The samples were under 1.0 MPa hydrostatic stress.
4.4 Permeability Variation due To Hydrostatic Stress

Fluid flow simulations were done for samples under changing hydrostatic stresses for the tests described in Section 3.3. A plot of stresses and permeability versus volumetric strain for an unbonded sample is shown in Figure 4.6. Permeability decreases with increasing stress almost linearly coming to a value 59% of the initial permeability value at the maximum stress of 5.4 MPa. As with the stresses, no hysteresis is observed in the permeability evolution during the unloading stage of the test; permeability increases along the same path during unloading.

Figure 4.7 shows a plot of hydrostatic stress and permeability versus volumetric strain for a weakly bonded sample. Permeability decreases with increasing volumetric strain (compaction); the reduction in permeability is approximately linear with volumetric strain. It is also linearly dependent on the hydrostatic stress up to the failure point at 17 MPa. Permeability decreases to 32% of its initial value at the end of compression test at a volumetric strain value of 4.6%, where the hydrostatic stress is 19 MPa. There is some hysteresis on the permeability as well during the unloading stage of the test. Permeability initially comes to higher values than it was at the same strain value during the unloading stage.

The permeability reduction in bonded samples agrees well both quantitatively and qualitatively with the experimental results of Dautriat et al. (2001). They observe a 40% reduction in permeability at 20 MPa on Bentheimer sandstone samples. Our results show a lower reduction in permeability than Sarda et al. (1999), who observe only a 20% reduction.
at 20 MPa. However their experiments were conducted on well consolidated sandstones. For comparison, the UCS of the rock samples they used was 120 MPa whereas our simulated samples had a UCS of 15 MPa. Qualitatively our results are similar to the experimental uniaxial strain tests of Soares et al. (2002). Their results show that the trend of permeability reduction with stress changes at a critical stress value, after which permeability decreases much faster with stress due to pore collapse.

The two main mechanisms for permeability reduction with increasing hydrostatic stress are the increase of normal forces between particles which increases the amount of normal overlap and the decrease in porosity due to particles coming closer together under the stresses. The increase in overlap causes a decrease in the pore throat radius as given by Equation 4.2. As seen in the Figure 4.9, the normal force chain network is much denser and thicker in higher hydrostatic stresses. By comparison the average normal contact force for a sample under a hydrostatic stress of 0.5 MPa is 8.1 Newton whereas for a sample under hydrostatic stress of 5.0 MPa the average normal contact force is 78.1 Newton. The reduction in porosity works similarly in both bonded and unbonded samples; however there is a larger permeability decrease due to hydrostatic stress in unbonded samples compared to bonded samples as seen in Figure 4.9. Permeability decreases up to 50% under 5.0 MPa in the case of unbonded samples whereas it decreases up to 5-10% in bonded samples. Unbonded samples get compacted more easily than bonded samples because there are no bonds to restrict the particles’ motion. Permeability decreases much faster after their bonds
break for the same hydrostatic stress increase, due to pore collapse and a fast decrease in porosity.

Figure 4.6: Permeability variation of an unbonded sample under hydrostatic compression test. $K_0=249$ D.
Figure 4.7: Permeability variation of a weakly bonded sample under hydrostatic compression test. $K_0=8.48$ D.

Figure 4.8: Permeability variation with hydrostatic stress for the two types of samples.
4.5 Permeability Variation during Triaxial Tests

Permeability variation of a sample during a triaxial test experiment is of particular interest. During the production of the hydrocarbons from the reservoir, fluid pressure decreases, whereas the value of the external stresses remain the same. This in turn induces changes in the effective stresses of the system. Rhett and Teufel (1992) show that the ratio $K$ of the change in horizontal stresses ($\Delta \sigma_h$) to the change in the vertical stresses ($\Delta \sigma_v$) is a constant and by virtue of Equation 1.1 the value of the differential stress increases while the pore pressure decreases. It is this increase in differential stress what we are simulating.
with the triaxial tests. In a triaxial test, vertical stress increases whereas the side (horizontal) stress is kept constant, increasing the value of the differential stress. As Dusseault (1997) and Oldakowski (1994) have shown, the deformation of a rock depends strongly on the stress path followed; hence we have also run simulations of radial extension experiments. In radial extension experiments the horizontal (side) stress decreases by making the sample expand in the horizontal direction. The vertical stress is kept constant which results in an increase in the value of the differential stress. In our simulations we measure both the permeability parallel to the higher stress, which in our case is the vertical permeability, $K_y$, and the permeability parallel to the lower stress, $K_x$.

Figure 4.10 shows the permeability variation (bottom) and differential stress versus axial strain of an unbonded sample during a triaxial test with a 0.35 MPa confining pressure. The sample is compressed to 6.4% axial strain value (loading), after which it the horizontal walls reverse their velocity (unloading stage). Horizontal permeability decreases by 13% initially until 1.2% axial strain after which it remains relatively constant until about 5% axial strain. The permeability parallel to the maximum stress $K_y$ on the other hand increases continuously during the loading stage of the test. The maximum value it reaches at 3.8% axial strain is 80% greater than the initial value. During the unloading stage of the test $K_x$ increases first by 45% and then remains relatively constant whereas $K_y$ increases up to 100% higher than initial value and then decreases to 65 % higher than the initial permeability at 3.2 % axial strain value.
Permeability variation (bottom) and differential stress versus axial strain of an unbonded sample during a triaxial test with a 1.0 MPa confining pressure is shown in Figure 4.11. Horizontal permeability decreases by 25% initially until 3% axial strain after which it increases and comes to the initial value at the end of compression stage of the test. $K_y$ on the other hand decreases up to 5% initially and then increases continuously during the loading stage of the test. The maximum value it reaches at 5.8% axial strain is 40% greater than the initial value. During the unloading stage of the test, $K_x$ increases even more and reaches to a value 40% higher than the initial permeability at the end of unloading stage of the test. $K_y$ remains relatively the same during the unloading stage of the test at a value 40% higher than the initial permeability.

Figure 4.12 shows the permeability variation (bottom) and differential stress versus axial strain of a weakly bonded sample during a triaxial test with a 0.35 MPa confining pressure. The sample is compressed vertically up to 3.2% axial strain value (loading), after which it the horizontal walls reverse their velocity (unloading stage). Both directional permeabilities decrease initially during the elastic portion of the stress-strain curve; $K_y$ starts to increase at the onset of brittle failure at 1.5 % axial strain and reaches 250% of the initial permeability at the end of loading stage of the test. $K_x$ on the other hand keeps decreasing even after brittle failure and reaches 50% of the initial permeability at 2% axial strain value, after which it starts to increase and ends being the same initial value at the end of the loading stage of the test. Both permeabilities continue to increase further during the unloading stage of the test. $K_x$ ends up 80% higher than the initial permeability. $K_y$, on the other hand increases seven fold the initial permeability.
This drastic increase in permeability can be explained micromechanically with the help of Figure 4.13. The figure shows the sample’s broken bonds, normal force chains and pore network at the end of the triaxial test as compared to those in the beginning of the test. As seen the bonds break with a preferred orientation, vertical direction, which in turns changes the microscopic force chain network of the sample and the pore network. Broken bonds cause the creation high conductivity channels in the vertical direction, which in turn increases the vertical permeability. It is the creation of these high conductivity channels in other bonded samples as well, that causes the increase in permeability after the sample fails.

Figure 4.14 shows the permeability variation (bottom) and differential stress versus axial strain of a weakly bonded sample during a triaxial test with a 1.5 MPa confining pressure. The sample is compressed vertically up to 3.2% axial strain value (loading), after which it the horizontal walls reverse their velocity (unloading stage). Both directional permeabilities decrease initially during the elastic portion of the stress-strain curve; $K_x$ decreasing by 60% at 3% axial strain value, whereas $K_y$ decreasing by 10% at 0.8% strain value. $K_y$ starts to increase at the onset of brittle failure at 1.5 % axial strain and reaches about 180% of the initial permeability at the end of loading stage of the test. $K_x$ on the other hand keeps decreasing even after brittle failure and reaches 45% of the initial permeability at 3% axial strain value, after which it starts to increase and ends 80% of initial value at the end of the loading stage of the test. $K_x$ continues to increase further during the unloading stage of the test and ends up 80% higher than the initial permeability. $K_y$, on the other hand increases initially during the unloading stage but then
decreases and ends up about the same as $K_Y$; about 80% higher than the value at the beginning of the test.

Permeability variation of the unbonded samples in triaxial test with confining pressure of 1.5 MPa agree qualitatively with the experimental results of Yaich (2008). Permeability decreases initially during the compaction/elastic portion of the stress strain curve. It starts to increase at the onset of dilatancy with a maximum 12% more than the initial value. Permeability variation of the weakly bonded samples agrees both qualitatively and quantitatively with the experimental results of Wang and Park (2002). Permeability of cemented sandstones they use in their triaxial test experiments decreases up to 30% during the elastic portion of the stress strain curve. At brittle failure permeability increases abruptly up to 2-3 times the initial value. Shao et al. (2005) also reports a permeability increase up to an order of magnitude during triaxial tests of brittle rocks.
Figure 4.10: Permeability variation (bottom) and differential stress (top) versus axial strain of an unbonded sample during 0.35 MPa confining stress triaxial test.
Figure 4.11: Permeability variation (bottom) and differential stress (top) versus axial strain of an unbonded sample during 1.0 MPa confining stress triaxial test.
Figure 4.12: Permeability variation (bottom) and differential stress (top) versus axial strain of a weakly bonded sample during 0.35 MPa confining stress triaxial test.
Figure 4.13: Particles and broken bonds, normal force chains and pore throat network for the bonded sample at the beginning of the low confining stress (0.35 MPa) triaxial sample and at the end of it.
Figure 4.14: Permeability variation (bottom) and differential stress (top) versus axial strain of a weakly bonded sample during 1.5 MPa confining stress triaxial test.
4.6 Permeability Variation during Failure due to Decreasing Confining Stress

To see the permeability variation on a bonded and unbonded sample on which the differential stress increases along a different stress path, we have simulated radial expansion tests and measured the permeability at different horizontal strain values. Directional permeabilities $K_x$ and $K_y$ are measured during the expansion and compressing back stages of the test. Two cases are studied for each type of sample, a lower initial hydrostatic stress and higher.

Figure 4.15 shows the permeability evolution (bottom) and stresses (top) versus horizontal strain during a radial expansion test of an unbonded sample with a 1.5 MPa initial hydrostatic stress. The side vertical walls move apart from each other (expansion stage) until a horizontal strain value of 2% is achieved, after which their velocities reverse (compaction) up to 1% horizontal strain value. Both directional permeabilities, $K_x$ and $K_y$ increase during the expansion stage of the test. $K_x$ increases 14% whereas $K_y$ increases by 54%. $K_y$ decreases during the compaction stage of the test, ultimately reaching a value only 20% higher than the initial permeability. $K_x$, on the other hand shows little variability during the compaction stage.

Results of a radial expansion test with a higher initial hydrostatic stress (5 MPa) on the same unbonded sample are shown in Figure 4.16. The permeability parallel to the maximum stress direction, $K_y$ increases continuously during the expansion stage of the test reaching 220% of the initial value at the end of the expansion stage, at 1.3% horizontal strain. $K_x$, on the other hand shows very little variation during the test; it increases about
10% at 0.8% horizontal strain. Both permeabilities decrease during the compaction phase of the test; $K_x$ coming back to the original value and $K_y$ coming to about 10% higher than the initial permeability at about 0.6% horizontal strain.

Figure 4.17 shows the permeability evolution (bottom) and stresses versus horizontal strain during a radial expansion test of a weakly unbonded sample with a 5.0 MPa initial hydrostatic stress. $K_x$ remains unaffected by the test both during the loading and the unloading stage of the test. $K_y$ on the other hand increases slowly initially, up to 20% higher than the initial value, at 3% horizontal strain value. At 3% horizontal strain, $K_y$ increases faster with horizontal strain, ending the expansion stage of the test at a value 280% of the initial value of the initial permeability value. It decreases following the same path as expansion during the compaction stage of the test, ending at a value 20% higher than the initial permeability.

Results of a radial expansion test with a higher initial hydrostatic stress (15 MPa) on the same weakly sample are shown in Figure 4.18. The permeability parallel to the maximum stress direction, $K_y$ increases continuously during the expansion stage of the test reaching a value 45% higher than the initial permeability value at 1.2% horizontal strain value. $K_x$, on the other hand decreases during the expansion stage of the test; it decreases by 12% at the end of the expansion stage of the test. Both permeabilities decrease during the compaction phase of the test; $K_x$ reaching 85% of the initial value and $K_y$ coming to about 12% higher than the initial permeability at about 0.6% horizontal strain.
Permeability variation of unbonded sample in radial expansion experiments agrees qualitatively with the experimental results of Yaich, 2008. A permeability increase of 40% is observed during radial expansion experiments with an initial isotropic stress of 200 Psia.
Figure 4.15: Permeability variation (bottom) and stresses (top) versus horizontal strain of an unbonded sample during radial expansion test. Initial hydrostatic stress is 1.5 MPa.
Figure 4.16: Permeability variation (bottom) and stresses (top) versus horizontal strain of an unbonded sample during radial expansion test. Initial hydrostatic stress is 5.0 MPa.
Figure 4.17: Permeability variation (bottom) and stresses (top) versus horizontal strain of a weakly bonded sample during radial expansion test. Initial hydrostatic stress is 5.0 MPa.
Figure 4.18: Permeability variation (bottom) and stresses (top) versus horizontal strain of a weakly bonded sample during radial expansion test. Initial hydrostatic stress is 15.0 MPa.
5 Summary

The discrete element method used is able to model the mechanical behavior of cemented and uncemented rock using relatively few input parameters. The parameters needed for the unbonded sample are 2-D porosity, particle’s stiffness, normal to shear stiffness ratio and the coefficient of friction. Porosity for the unbonded samples is decided as the lowest value which gives a very low isotropic stress after particle generation and the maximum unbalanced forces are reduced to 1% of the average contact forces between particles. Particle stiffness, which controls the macroscopic Young’s modulus of the sample, is fitted to experimental data done on uncemented sands. The friction coefficient, which controls the maximum stress value before dilatancy is also fitted to experimental data from triaxial tests performed on uncemented sands. Values fitting the experimental data for the particle elastic Young’s modulus and friction coefficient are 0.21 GPa and 0.8 respectively. The normal to shear stiffness ratio which controls the Poisson’s ration of the sample during a triaxial test, is assigned a value of 5. The unbonded sample has a macroscopic bulk modulus of 112 MPa during hydrostatic loading and a Young’s modulus of 81 MPa during triaxial tests. It endures a maximum stress of 1.2 MPa during 0.35 MPa confining pressure triaxial tests. The value of the maximum stress the unbonded sample endures during triaxial tests increases linearly with confining pressure. Radial (horizontal) expansion test results on unbonded sample reveal that horizontal stress decreases linearly up to a horizontal strain value after which it remains relatively constant due to shear failure. Path hysteresis in stress and strains is always observed after shear failure in all nonhydrostatic tests performed on the unbonded samples.
Porosity for the weakly bonded samples on the other hand is 0.15. This value for porosity gives a value of about 3 MPa isotropic stress after particle generation. The values for the particle stiffness, coefficient of friction and normal to shear stiffness ratio are the same as those of the unbonded sample. The extra parameters for the weakly bonded samples are related to the parallel bonds. Since the cementation in most cemented rocks is of the same mechanical properties as the grains themselves, the stiffness of the bonds is assigned a value of 75% of particle’s stiffness in our simulations. Both the bond size and bond strength determine the strength of the bonded sample. The criterion in our case is the unconfined compressive strength. Unconfined compressive strength increases with both bond size and bond strength. A value of bond size multiplier of 0.5 and a value for both shear and tensile strength of 15 MPa is assigned for the weakly bonded sample. With these parameters the weakly bonded sample has an unconfined compressive strength of 15.4 MPa, a Young modulus of 1.1 GPa during triaxial tests, and an elastic bulk modulus of 0.67 GPa. Bonds break in a preferred direction during brittle failure in triaxial and unconfined compressive tests on weakly bonded samples. The preferred direction is diagonal to the sample. Tension induced broken bonds dominate at low confining stresses, whereas shear induced bonds become abundant at higher confining stresses. Pore collapse occurs during hydrostatic loading tests on the weakly bonded sample. For our simulated weakly bonded sample pore collapse happens at a value of 17 MPa hydrostatic stress. Pore collapse is evident in a change of slope in the hydrostatic stress-volumetric curve; a greater change in volumetric strain for the same hydrostatic stress increase. The weakly bonded sample fails in a brittle way at unconfined compressive tests and at low confining pressure
triaxial experiments. However at high confining pressure triaxial tests, it fails in a ductile, strain hardening way. The threshold value for the confining pressure where the change in the behavior occurs for our simulated weakly bonded sample is about 4 MPa. Radial (horizontal) expansion test results on weakly bonded sample reveal that horizontal stress decreases linearly up to a horizontal strain value after which it remains relatively constant due to shear failure. Path hysteresis in stress and strains is always observed after failure in all nonhydrostatic tests performed on the unbonded samples. There is also hysteresis in stress in the hydrostatic compressing test after pore collapse. The weakly bonded sample’s mechanical properties are altered after failure.

Permeability variation of unbonded and weakly bonded samples is observed in hydrostatic compressing, triaxial and radial extension tests. Permeability variation depends strongly on the type of mechanical test performed on the sample. The greatest permeability reduction in unbonded samples is observed during hydrostatic compression tests; a drop of 43% in permeability is observed at 5.4 hydrostatic pressure. A maximum reduction of about 60% in weakly bonded sample’s permeability is observed during hydrostatic compression test at 20 MPa hydrostatic stress, and during 1.5 MPa confining pressure triaxial test. The deviatoric stress was about 10 MPa in the case the triaxial test. Permeability decreases at a rate of about 2% per MPa hydrostatic pressure in weakly bonded samples before pore collapse pressure (17 MPa) after which the permeability decreases much faster with hydrostatic pressure. Permeability variation follows the same trend as stress variation during hydrostatic compression experiments. It decreases linearly
with volumetric strain during the elastic portion of the stress-strain curve, the trend changes when pore collapse occurs.

There is variation in both vertical (axial) and horizontal (radial) permeabilities during both triaxial and radial expansion tests in unbonded samples. At higher confining pressure (1.0 MPa) triaxial tests both horizontal and vertical permeability decrease during the elastic compression portion of the stress strain curve. $K_x$ decreases up to 40%, whereas $K_y$ decreases by 5%. In the case of lower confining pressure (0.35 MPa) triaxial tests, the unbonded sample’s vertical permeability increases even during the compressive, elastic portion of the stress strain curve. At shear failure unbonded samples’ both vertical and horizontal permeability increases. A 100% increase in $K_y$ is observed with 0.35 MPa confining pressure triaxial test in the unbonded sample, and a 40% increase in the case of 1.5 MPa confining pressure. $K_x$, on the other hand increases up to 40% in the case of 0.35 MPa confining pressure triaxial test and comes to the initial value in the case of 1.0 MPa confining pressure test.

There is a reduction in the permeability of weakly bonded samples initially during triaxial tests, in both low (0.35 MPa) and high (1.5 MPa) confining pressure cases. Horizontal permeability drops by 40% and vertical permeability $K_y$ drops by 5% initially during the elastic portion of the stress strain curve in the 0.35 MPa confining stress triaxial test. $K_x$ decreases by 60% during and $K_y$ by 10% during the 1.5 MPa confining stress triaxial test. It is interesting to note that $K_x$ decreases even after brittle failure in the case of 1.5 MPa confining stress triaxial test and stats increasing only at a higher strain value. The
60% reduction in $K_x$ during the triaxial test at about 10 MPa deviatoric stress is comparable to the 60% decrease during the hydrostatic loading. There is path hysteresis in permeability as well during the unloading stage of the triaxial tests for both unbonded and bonded samples. $K_x$ of the unbonded sample increases during the unloading stage at 1.0 MPa confining pressure and it remains relatively unchanged at 0.35 MPa confining pressure triaxial tests. $K_y$ of the unbonded sample, on the other hand decreases during the unloading stage at 0.35 MPa confining pressure and remains relatively unchanged at 1.0 MPa confining pressure triaxial tests.

Both directional permeabilities of the unbonded sample, $K_x$ and $K_y$ increase during the radial expansion test with a 1.5 MPa initial hydrostatic pressure. $K_x$ increases up to 15%, whereas $K_y$ increases 55% at the end of expansion stage of the test. Horizontal permeability remains relatively unaltered during the expansion stage in the case of 5 MPa initial hydrostatic pressure radial expansion test. Vertical permeability $K_y$, on the other hand increases by 130% at the end of expansion stage. Directional permeabilities decrease during the compression stage of the test for both cases. However there is path hysteresis, just as the path hysteresis in the stresses and strains.

Horizontal permeability of the weakly bonded sample is constant during the radial expansion test with 5 MPa initial hydrostatic pressure. Vertical permeability increases slowly at first, then faster and reaches a value 180% larger than the initial value. Horizontal permeability decreases slightly by 10% during 15 MPa initial hydrostatic pressure radial expansion test. Vertical permeability on the other hand increases up to 45%. There is very
little path hysteresis in permeability evolution during the compression stage of the test for the lower initial hydrostatic (5 MPa) pressure test. There is noticeable path hysteresis in the case of \( K_y \) during the compressive stage of the 15 MPa initial hydrostatic pressure test. \( K_x \) on the other hand decreases even further, up to 20 % of its initial value.

The results show that permeability of uncedented and weakly cemented sands are closely related to the stress state and micromechanics of the system. The trend of change in permeability changes at the same point with the change in trend of stress-strain curve of the system. Permeability varies with stress but is dependent not only on the stress state of the system but also with the stress path as seen in our different results with different mechanical tests. Whenever there is stress path hysteresis there is also permeability path hysteresis, which indicates a strong coupling. One of the mechanisms responsible for the permeability variation in our modeled samples is the change in pore and pore throat size due to compression. The reduction of pore and pore throat size reduces permeability, with a more pronounced effect in uncedented sands. Another mechanism is the creation of high conductivity channels and fractures with a preferred direction during failure. The creation of these fractures is more effective in low confining stresses when the highest increase in permeability is observed. At higher confining stresses the effect is reduced.
6 Bibliography


7 Appendix

The following FISH file codes used in PFC-2D were modified from example files provided by Itasca with the software.

Sample Generation File:

```plaintext
new
set disk on
def setup ; Initialize user variables
x_min=-0.04
x_max=0.04
y_min=-0.04
y_max=0.04
E=3.0e9; 3.0e9 ; 3.0e9 ;
lo_rad=0.0004
hi_rad=0.0006
poros=0.17; 0.16 ; 0.17,
n_stiff=2*E
kn_ks_ratio=2
s_stiff=n_stiff / kn_ks_ratio
n_stiffw=n_stiff*1; 0.0
s_stiffw=n_stiffw
n_stiffx=n_stiff
s_stiffx=n_stiffx/kn_ks_ratio
 Nx=1.2*x_max/(lo_rad+hi_rad)
Ny=Nx*y_max/x_max
r_s=0.0003
r_s1=r_s*0.5
nball=4*y_max*x_max*(1-poros)/(3.14*r_s*r_s)
_fric= 0.8
bond_mult = 1.0
bkn=90.0e6;
bks= bkn
belk=0.5*E/(bond_mult*0.5*(lo_rad+hi_rad)) ; n_stiff
belx=belk /kn_ks_ratio
meas_rad = x_max*0.75
end
setup
def make_model
;--- Derived and internal data ---
a_sum  = (x_max - x_min) * (y_max - y_min)
rmult = 1.5
rmean=0.5*(hi_rad+lo_rad)
amean = pi * (hi_rad^3 - lo_rad^3) / (3.0*(hi_rad-lo_rad))
nball = (1.0 - poros) * a_sum / amean
r1red = lo_rad / rmult
r2red = hi_rad / rmult
```
x_min2=x_min*1.0
x_max2=x_max*1.0
y_min2=y_min*1.0
y_max2=y_max*1.0
nball1=nball/10
nball2=nball1+1
nball3=2*nball/10
nball4=nball3+1
nball5=3*nball/10
nball6=nball5+1
nball7=4*nball/10
nball8=nball7+1
nball9=5*nball/10
nball10=nball9+1
nball11=6*nball/10
nball12=nball11+1
nball13=7*nball/10
nball14=nball13+1
nball15=8*nball/10
nball16=nball15+1
nball17=9*nball/10
nball18=nball17+1
nex1=nball+1
nex2=nex1+0.055*nball
nex3=nex2+1
nex4=nex3+0.055*nball
nex5=nex4+1
nex6=nex5+0.05*nball
nex7=nex6+1
nex8=nex7+0.05*nball
y_m1=y_min+(y_max-y_min)/10
y_m2=y_min+2*(y_max-y_min)/10
y_m3=y_min+3*(y_max-y_min)/10
y_m4=y_min+4*(y_max-y_min)/10
y_m5=y_min+5*(y_max-y_min)/10
y_m6=y_min+6*(y_max-y_min)/10
y_m7=y_min+7*(y_max-y_min)/10
y_m8=y_min+8*(y_max-y_min)/10
y_m9=y_min+9*(y_max-y_min)/10

;--- Create assembly ---
command
wall id=1 ks=n_stiffw kn=n_stiffw nodes x_min2,y_min2 x_max2,y_min2
wall id=2 ks=n_stiffw kn=n_stiffw nodes x_max2,y_min2 x_max2,y_max2
wall id=3 ks=n_stiffw kn=n_stiffw nodes x_max2,y_max2 x_min2,y_max2
wall id=4 ks=n_stiffw kn=n_stiffw nodes x_min2,y_max2 x_min2,y_min2
gen no_shad id=1,nball1 x=x_min,x_max y=y_min,y_m1 rad=r1red,r2red tries 10000000
prop dens 2600 ks=s_stiff kn=n_stiff
gen no_shad id=nball2,nball3 x=x_min,x_max y=y_m1,y_m2 rad=r1red,r2red tries 10000000
prop dens 2600 ks=s_stiff kn=n_stiff
gen no_shad id=nball4,nball5 x=x_min,x_max y=y_m2,y_m3 rad=r1red,r2red tries 10000000
prop dens 2600 ks=s_stiff kn=n_stiff
gen no_shad id=nball6,nball7 x=x_min,x_max y=y_m3,y_m4 rad=r1red,r2red tries 10000000
prop dens 2600 ks=s_stiff kn=n_stiff
prop dens 2600 ks=s\_stiff kn=n\_stiff

`gen no\_shad  id=nball8,nball9  x=x\_min,x\_max  y=y\_m4,y\_m5  rad=r1red,r2red  tries 10000000`

prop dens 2600 ks=s\_stiff kn=n\_stiff

`gen no\_shad  id=nball10,nball11  x=x\_min,x\_max  y=y\_m5,y\_m6  rad=r1red,r2red  tries 10000000`

prop dens 2600 ks=s\_stiff kn=n\_stiff

`gen no\_shad  id=nball12,nball13  x=x\_min,x\_max  y=y\_m6,y\_m7  rad=r1red,r2red  tries 10000000`

prop dens 2600 ks=s\_stiff kn=n\_stiff

`gen no\_shad  id=nball14,nball15  x=x\_min,x\_max  y=y\_m7,y\_m8  rad=r1red,r2red  tries 10000000`

prop dens 2600 ks=s\_stiff kn=n\_stiff

`gen no\_shad  id=nball16,nball17  x=x\_min,x\_max  y=y\_m8,y\_m9  rad=r1red,r2red  tries 10000000`

prop dens 2600 ks=s\_stiff kn=n\_stiff

`gen no\_shad  id=nball18,nball  x=x\_min,x\_max  y=y\_m9,y\_max  rad=r1red,r2red  tries 10000000`

prop dens 2600 ks=s\_stiff kn=n\_stiff

`;gen no\_shad  id=nex1,nex2  x=x\_min2,x\_min  y=y\_min2,y\_max2  rad=r1red,r2red  tries 10000000`

`;prop dens 2600 ks=s\_stiff kn=n\_stiff`

`;gen no\_shad  id=nex3,nex4  x=x\_max,x\_max2  y=y\_min2,y\_max2  rad=r1red,r2red  tries 10000000`

`;prop dens 2600 ks=s\_stiff kn=n\_stiff`

`;gen no\_shad  id=nex5,nex6  x=x\_min,x\_max  y=y\_min2,y\_min  rad=r1red,r2red  tries 10000000`

`;prop dens 2600 ks=s\_stiff kn=n\_stiff`

`;gen no\_shad  id=nex7,nex8  x=x\_min,x\_max  y=y\_max,y\_max2  rad=r1red,r2red  tries 10000000`

`;prop dens 2600 ks=s\_stiff kn=n\_stiff`

ini rad mul rmult
endcommand

end

make\_model

set dt dscale

cyc 20000

solve

range name r1 id 1, nball1
range name r2 id nball2, nball3
range name r3 id nball4, nball5
range name r4 id nball6, nball7
range name r5 id nball8, nball9
range name r6 id nball10, nball11
range name r7 id nball12, nball13
range name r8 id nball14, nball15
range name r9 id nball16, nball17
range name r10 id nball18, nball
range name r\_all id 1,nball
range name r\_ex id nex1,nex8
meas id 13 x 0 y 0 rad meas\_rad
hist id 121 meas poros id 13
hist id 131 meas s11 id 13
hist id 132 meas s22 id 13
plot create __stress
plot hist -131 -132
plo show
plot create __poros
plo hist 121
plo sho

;-----------------------------FISHCALL
call fishcall.fis

;------------------------CRACK TRACKING
set dt dscale
solve
del wall 11
del wall 22
del wall 33
del wall 44
def colorz
nn1 = NN/10
nn2 = 2*NN/10
nn3 = 3*NN/10
nn4 = 4*NN/10
nn5 = 5*NN/10
nn6 = 6*NN/10
nn7 = 7*NN/10
nn8 = 8*NN/10
nn9 = 9*NN/10
end
colorz
range name r1 id 1, nbll1
range name r2 id nbll2, nbll3
range name r3 id nbll4, nbll5
range name r4 id nbll6, nbll7
range name r5 id nbll8, nbll9
range name r6 id nbll10, nbll11
range name r7 id nbll12, nbll13
range name r8 id nbll14, nbll15
range name r9 id nbll16, nbll17
range name r10 id nbll18, nbll
range name r_all id 1,nbll
range name r_ex id nex1,nex8
plot create qqq
plot add ball yellow range r1
plot add ball cyan range r2
plot add ball white range r3
plot add ball brown range r4
plot add ball yellow range r5
plot add ball cyan range r6
plot add ball white range r7
plot add ball brown range r8
plot add ball yellow range r9
plot add ball cyan range r10
plot add ball black range r_ex
plot add wall black
;plot show
prop pb_rad bond_mult pb_kn belk pb_ks bels pbnstrength bkn pb_sstrength bks range r_all
prop fric_fric range r_all
;prop fric 0 range r_ex
set dt dscale
solve
save sample.sav
Servo Mechanism File:

;FILE NAME: servo.data
new
rest sample.sav
del wall 1
del wall 3
del wall 2
del wall 4

def build_walls

\[ x_{\text{min}1} = x_{\text{min}2} \times 1.0/2;5 \]
\[ x_{\text{max}1} = x_{\text{max}2} \times 1.0/2;05 \]
\[ y_{\text{min}1} = y_{\text{min}2} \times 1.0/2;05 \]
\[ y_{\text{max}1} = y_{\text{max}2} \times 1.0/2;05 \]
\[ x_{\text{min}w} = x_{\text{min}} \times 1.5 \]
\[ y_{\text{min}w} = y_{\text{min}} \times 1.2 \]
\[ y_{\text{max}w} = y_{\text{max}} \times 1.2 \]
\[ \text{meas rad} = 0.6 \times x_{\text{max}} \]

\text{command}

wall id=5 kn=n_{\text{stiffw}} ks=n_{\text{stiffw}} nodes x_{\text{min}w},y_{\text{min}1} x_{\text{max}w},y_{\text{min}1}
wall id=6 kn=n_{\text{stiffw}} ks=n_{\text{stiffw}} nodes x_{\text{max}1},y_{\text{min}w} x_{\text{max}1},y_{\text{max}w}
wall id=7 kn=n_{\text{stiffw}} ks=n_{\text{stiffw}} nodes x_{\text{max}w},y_{\text{max}1} x_{\text{min}w},y_{\text{max}1}
wall id=8 kn=n_{\text{stiffw}} ks=n_{\text{stiffw}} nodes x_{\text{min}1},y_{\text{max}w} x_{\text{min}1},y_{\text{min}w}
end_command

end

build_walls

plot create SAMPLE
plo add wall black
plot add ball yellow range r1
plot add ball cyan range r2
plot add ball white range r3
plot add ball brown range r4
plot add ball yellow range r5
plot add ball cyan range r6
plot add ball white range r7
plot add ball brown range r8
plot add ball yellow range r9
plot add ball cyan range r10
plot add ball black range r_ex
/plot add vel red
/plot show
solve
macro zero 'ini xvel 0 yvel 0 spin 0'
def get_ss ; determine average stress and strain at walls
\[ \text{xdif} = w_{x(wadd6)} - w_{x(wadd8)} \]
\[ \text{ydif} = w_{y(wadd7)} - w_{y(wadd5)} \]
new_xwidth = xdif+2*x_max2
new_height = ydif+2*y_max2
wsxx = 0.5 * (w_xfob(wadd8) - w_xfob(wadd6)) / (new_height * 1.0)
wsyy = 0.5 * (w_yfob(wadd5) - w_yfob(wadd7)) / (new_xwidth * 1.0)
dev = wsyy - wsxx
wexx = xdif / (new_xwidth) - wexx0
weyy = ydif / (new_height) - weyy0
wevol = xdif / (new_xwidth) + ydif / (new_height) - wexx0 - weyy0
end

def get_gain ; determine servo gain parameters for x and y
  alpha = 0.5 ; relaxation factor
  count = 0
  avg_stiff = 0
  cp = contact_head ; find avg. number of contacts on x-walls
    loop while cp # null
      if c_ball1(cp) = wadd6
        count = count + 1
        avg_stiff = avg_stiff + c_kn(cp)
      end_if
      if c_ball1(cp) = wadd8
        count = count + 1
        avg_stiff = avg_stiff + c_kn(cp)
      end_if
      if c_ball2(cp) = wadd6
        count = count + 1
        avg_stiff = avg_stiff + c_kn(cp)
      end_if
      if c_ball2(cp) = wadd8
        count = count + 1
        avg_stiff = avg_stiff + c_kn(cp)
      end_if
      cp = c_next(cp)
    end_loop
  nxcount = count / 2.0
  if count = 0
    avg_stiff = 0
  else
    avg_stiff = avg_stiff / count
  end_if
  if count<6
    gx = -(2*strain_rate*x_max1)/sxxreq
  else
    gx = alpha * (y_max * 2.0) / (avg_stiff * nxcount*tdel)
  end_if
  count = 0
  avg_stiff = 0
  cp = contact_head ; find avg. number of contacts on y-walls
    loop while cp # null
      if c_ball1(cp) = wadd5
        count = count + 1
      end_if
      if c_ball1(cp) = wadd7
        count = count + 1
      end_if
      cp = c_next(cp)
    end_loop
  end_def

end
avg_stiff = avg_stiff + c_kn(cp)
end_if
if c_ball1(cp) = wadd7
count = count + 1
avg_stiff = avg_stiff + c_kn(cp)
end_if
if c_ball2(cp) = wadd5
count = count + 1
avg_stiff = avg_stiff + c_kn(cp)
end_if
if c_ball2(cp) = wadd7
count = count + 1
avg_stiff = avg_stiff + c_kn(cp)
end_if
cp = c_next(cp)
end_loop
nycount = count / 2.0
if count=0
avg_stiff=0
else
avg_stiff = avg_stiff / count
end_if
if count<12
gy=-(2*strain_rate*y_max1)/syyreq
else
gy = alpha * (x_max1 * 2.0) / (avg_stiff*nycount*tdel)
end_if
end
def servo
while_stepping
get_ss ; compute stresses & strains
if XX=1
udx = gx * (wsxx - sxxreq)
end_if
if XX=0
udx=-2*strain_rate*x_max
end_if
if XX=2
udy=0
end_if
if YY=1
udy = gy *(wsyy-syyreq)
end_if
if YY=0
udy = 2*strain_rate*y_max
end_if
if YY=2
udy=0
end_if
w_xvel(wadd8) = udx
w_xvel(wadd6) = -udx
w_yvel(wadd5) = udy
w_yvel(wadd7) = -udy
end
def wall_addr
wadd5 = find_wall(5)
wadd6 = find_wall(6)
wadd7 = find_wall(7)
wadd8 = find_wall(8)
end
def iterate
loop while 1 ≠ 0
  get_gain
  servo
  if (abs((wsxx - sxxreq)/sxxreq)+abs((wsyy-syyreq)/syyreq)) < sig_tol then
    weyy0=weyy
    wexx0=wexx
    exit
    end_if
    command
    zero
    solve
    end_command
  end_loop
end
def iteratex
loop while 1 ≠ 0
  get_gain
  servo
  if (abs((wsxx - sxxreq)/sxxreq)) < sig_tol then
    exit
    end_if
    command
    zero
    solve
    end_command
  end_loop
end
def iteratey
loop while 1 ≠ 0
  get_gain
  servo
  if (abs((wsyy - syyreq)/syyreq)) < sig_tol then
    exit
    end_if
    command
    zero
    solve
    end_command
  end_loop
end
SET sxxreq= -5.0e6  syyreq= -5.0e6  sig_tol=0.01  YY=1  XX=1
SET strain_rate=1e-6
set hist_rep 20
hist id 11 wsxx get_ss
hist id 15 wsyy get_ss
hist id 17 udx servo
hist id 18 udy servo
plot create STRESSES
plot hist -11 -15
;plot show
zero
wall_addr
iterate ; get all stresses to requested state
;hist write -11 -15 17 18  file ssss.data
set YY=2  XX=2
cyc 10
save servoed_sample.SAV
return

Fluid Flow Domain Building File:

;FILE NAME: DOM.data
new
;--- domain scan ... build up data structure
set echo on
res servoed_sample.sav; ystress2.sav ;

prop n_bond 1e10 s_bond 1e10
set extra contact 5
plo mod 1 red lred yell

def get_dom_mem; Return pointer to new domain object
   pnt = get_mem(dom_size)
   if pnt = null
      error = 'memory unavailable for domain item'
      endif
   mem(pnt) = dom_head
   dom_head = pnt
   mem(pnt+1) = null
   get_dom_mem = pnt
end
def dom_scan ; Create domains (list of voids between balls
;--- Number of items in domain object ---
dom_size = 8
;--- Symbols for domain offsets ...
DOM_LINK = 0 ; Link (always zero)
DOM_BALL_LIST = 1 ; Pointer to list of balls comprising domain
 ; ( list of doubles: (LINK,B_POINT) )
DOM_X = 2 ; X coordinate (not updated automatically)
DOM_Y = 3 ; Y coordinate
DOM_PRESS = 4 ; Pressure
DOM_VSUM = 5 ; Flow volume-sum
DOM_VOL = 6 ; Domain volume
DOM_FIX = 7 ; Fix flag (=1 if pressure fixed)
dom_head = null
;--- Number of items in flow object (extension to contact) ---
flow_size = 5
FLOW_DOM1 = 1 ; Pointer to domain 1
FLOW_DOM2 = 2 ; Pointer to domain 2
FLOW_AP_ZERO = 3 ; Residual aperture
FLOW_PERM = 4 ; Permeability constant
FLOW_ACTIVE = 5 ; = 1 if pipe is active; else 0
;--- Symbols for domain offsets ...
;--- (domains scan won't work if dead ends exist)
zap_dead_ends
;--- Initialize container to store domain links ---
; #1 = D pointer corresponding to path B1->B2
; #2 = D pointer corresponding to path B2->B1
cp = contact_head
loop while cp # null
c_extra(cp,FLOW_DOM1) = null
c_extra(cp,FLOW_DOM2) = null
c_extra(cp,FLOW_AP_ZERO) = 0.0
c_extra(cp,FLOW_PERM) = 0.0
c_extra(cp,FLOW_ACTIVE) = 0
endLoop
scan_all_contacts ; (do twice, to get both senses)
scan_all_contacts
pnt = dom_head ; Mark the outer domain
count_max = 0
outer_domain = null
loop while pnt # null
count = 0
bp = mem(pnt+1)
loop while bp # null
count = count + 1
bp = mem(bp)
endLoop
if count > count_max
count_max = count
outer_domain = pnt
endif
pnt = mem(pnt)
def domains ; Domain printout    count = 0
   pnt = dom_head
   loop while pnt # null
      if pnt # outer_domain
         count = count + 1
         oo = out(' Domain '+string(count)+'.  Balls are ...')
         iadd = mem(pnt+1)
         loop while iadd # null
            oo = out('            '+string(b_id(mem(iadd+1))))
            iadd = mem(iadd)
         endloop
      endif
      pnt = mem(pnt)
   endloop
   domains = count
end

def scan_all_contacts;--- Scan contacts, to form domains ---
cpstart = contact_head
loop while cpstart # null
   section
      if c_bflag(cpstart) = 0
         exit section
      endif
      cp = cpstart
      b1 = c_ball1(cp)
      b2 = c_ball2(cp)
      if c_extra(cp,FLOW_DOM2) # null ; (choose unused path)
         if c_extra(cp,FLOW_DOM1) # null
            exit section
         else
            bstart = b2
            va1 = c_xun(cp)
            va2 = c_yun(cp)
            dom_pnt = get_dom_mem
            c_extra(cp,FLOW_DOM1) = dom_pnt
         endif
      else
         bstart = b1
         va1 = -c_xun(cp)
         va2 = -c_yun(cp)
         dom_pnt = get_dom_mem
         c_extra(cp,FLOW_DOM2) = dom_pnt
      endif
      b2 = bstart
      loop nnn (1,1000) ; (hope outer domain < 1000 balls)
         ;-- scan contacts on next ball for max angle
         max_angle = -1e20
         cp_next = null
      endloop
   endsection
endloop

endLoopp
oo = out('Outer domain has '+string(count_max)+' balls')
end
next_ball = null
_cp = b_clist(b2)
loop while _cp # null
  _b1 = c_ball1(_cp)
  _b2 = c_ball2(_cp)
  if c_bflag(_cp) # 0
    if _cp # cp ; (don't take entry contact)
      if _b1 = b2
        vb1 = c_xun(_cp)
        vb2 = c_yun(_cp)
        next_poss = _b2
        flag = 1
      else
        vb1 = -c_xun(_cp)
        vb2 = -c_yun(_cp)
        next_poss = _b1
        flag = 0
      endif
    cc = va1*vb2 - va2*vb1 ; Cross product
    maga = sqrt(va1*va1 + va2*va2)
    na1 = va1 / maga
    na2 = va2 / maga
    bb = vb1*na1 + vb2*na2 ; Dot product
    dthet = atan2(abs(cc),bb^2)
    if cc > 0.0
      if bb < 0.0
        dthet = pi - dthet
      endif
    else
      if bb > 0.0
        dthet = -dthet
      else
        dthet = dthet - pi
      endif
    endif
    if dthet > max_angle
      max_angle = dthet
      cp_next = _cp
      next_ball = next_poss
      v1sav = vb1
      v2sav = vb2
      flagsav = flag
    endif
  endif
  if _b1 = b2
    _cp = c_b1clist(_cp)
  else
    _cp = c_b2clist(_cp)
  endif
endLoop
if flagsav = 1
c_extra(cp_next,FLOW_DOM1) = dom_pnt
else
c_extra(cp_next,FLOW_DOM2) = dom_pnt
endif
add_ball_to_domain
if next_ball = bstart
exit section
endif
b2 = next_ball
cp = cp_next
va1 = v1sav
va2 = v2sav
end_loop
;--- end of main contact scan ---
endSection

endLoop

deffzap_dead_ends
;--- Eliminate balls with one or less contacts ---

loop nnn(1,20)
num_zapped = 0
bp = ball_head
loop while bp # null
next = b_next(bp)
count = 0
cp = b_clist(bp)
loop while cp # null
if c_bflag(cp) # 0
   count = count + 1
endif
b1 = c_ball1(cp)
b2 = c_ball2(cp)
if b1 = bp
   cp = c_b1clist(cp)
else
   cp = c_b2clist(cp)
endif
endLoop
if count <= 1
   oo = del_ball(bp)
   num_zapped = num_zapped + 1
endif
bp = next
endLoop
if num_zapped > 0
   oo = out('Number of balls removed = ' + string(num_zapped))
else
   exit
endif
endLoop
def add_ball_to_domain; INPUT: dom_pnt, next_ball
  pnt = get_mem(2)
  if pnt = null
    error = 'no memory for ball double'
  endif
  mem(pnt) = mem(dom_pnt+1)
  mem(dom_pnt+1) = pnt
  mem(pnt+1) = next_ball
end

def set_dom_coords; set coordinates for domain centers; INPUT: dom = domain pointer
  iadd = mem(dom+DOM_BALL_LIST)
  xav = 0.0
  yav = 0.0
  count = 0
  loop while iadd # null
    bp = mem(iadd+1)
    xav = xav + b_x(bp)
    yav = yav + b_y(bp)
    count = count + 1
    iadd = mem(iadd)
  endloop
  xav = xav / count
  yav = yav / count
  mem(dom+DOM_X) = xav ; side-effect!
  mem(dom+DOM_Y) = yav
end

def dom_item; Plot item for domains
  array vec(dim) v1(dim) v2(dim)
  plot_item
  oo = set_color(0)
  pnt = dom_head
  loop while pnt # null
    if pnt # outer_domain
      dom = pnt
      set_dom_coords
      vec(1) = mem(pnt+DOM_X)
      vec(2) = mem(pnt+DOM_Y)
      oo = fill_circle(vec,0.00002)
    endif
    pnt = mem(pnt)
  endloop
plot_item
  oo = set_color(0)
  pnt = dom_head
  loop while pnt # null
    if pnt # outer_domain
      dom = pnt
      set_dom_coords
      vec(1) = mem(pnt+DOM_X)
      vec(2) = mem(pnt+DOM_Y)
      oo = fill_circle(vec,0.00002)
    endif
    pnt = mem(pnt)
  endloop
plot_item
  oo = set_line_width(1)
  cp = contact_head
  loop while cp # null
    if c_bflag(cp) # 0
      oo = set_color(1)
      b1 = c_ball1(cp)
      b2 = c_ball2(cp)
v1(1) = b_x(b1)
v1(2) = b_y(b1)
v2(1) = b_x(b2)
v2(2) = b_y(b2)
oo = draw_line(v1,v2)
endif
if c_extra(cp,FLOW_ACTIVE) = 1
  dom1 = c_extra(cp,FLOW_DOM1)
dom2 = c_extra(cp,FLOW_DOM2)
  if dom1 # null
    oo = set_color(0)
v1(1) = mem(dom1+2)
v1(2) = mem(dom1+3)
v2(1) = mem(dom2+2)
v2(2) = mem(dom2+3)
oo = draw_line(v1,v2)
  endif
endif
  cp = c_next(cp)
endloop
oo = set_line_width(0)
end
def set_active_flag ; ... on contacts for which flow is calculated
  cp = contact_head
loop while cp # null
  dom1 = c_extra(cp,FLOW_DOM1)
dom2 = c_extra(cp,FLOW_DOM2)
  if dom1 # null
    if dom2 # null
      if dom1 # outer_domain
        if dom2 # outer_domain
          c_extra(cp,FLOW_ACTIVE) = 1
        endif
      endif
    endif
  endif
cp = c_next(cp)
endloop
end
set echo on
dom_scan
set_active_flag
plo add fish dom_item green white
prop n_bond 0 s_bond 0
save dom_perm.sav

Fluid Flow and Permeability Simulation File:
res dom_perm.sav
set echo on

def pressure
    plot_item
    array pvec(dim)

    ;--- plot pressures as filled circles with various radii ---
    ; First, get max pressure ..
    press_max = 0.0
    pnt = dom_head
    loop while pnt # null
        if pnt # outer_domain
            press_max = max(press_max,mem(pnt+DOM_PRESS))
        endif
        pnt = mem(pnt)
    endloop
    if press_max = 0.0
        exit
    endif
    pnt = dom_head
    loop while pnt # null
        if pnt # outer_domain
            dom = pnt
            set_dom_coords
            vec(1) = mem(pnt+DOM_X)
            vec(2) = mem(pnt+DOM_Y)
            rad = 0.8*lo_rad * mem(pnt+DOM_PRESS) / press_max
            if rad > 0.000001
                oo = fill_circle(vec,rad)
            endif
        endif
        pnt = mem(pnt)
    endloop
end

def flow_props ; Set properties for flow calc
    cp = contact_head
    loop while cp # null
        if c_extra(cp,FLOW_DOM1) # null
            c_extra(cp,FLOW_AP_ZERO) = ap_zero
            c_extra(cp,FLOW_PERM) = perm
        endif
        cp = c_next(cp)
    endLoop
end

def flow_run ; Run flow calculation
    while_stepping
        n_rep = n_rep + 1
        if n_rep < 10

127
exit
endif
n_rep=0

;--- Flow in pipes ...
q_tot1=0.0
q_tot2=0.0
q_tot3=0.0
q_tot4=0.0
cmp = contact_head
loop while cp # null
  if c_extra(cp,FLOW_ACTIVE) = 1
    b1 = c_ball1(cp)
b2 = c_ball2(cp)
    rsum = b_rad(b1) + b_rad(b2)
    dom1 = c_extra(cp,FLOW_DOM1)
    dom2 = c_extra(cp,FLOW_DOM2)
    xx1=mem(dom1+DOM_X)
    xx2=mem(dom2+DOM_X)
    yy1=mem(dom1+DOM_Y)
    yy2=mem(dom2+DOM_Y)
    pdiff = mem(dom1+DOM_PRESS) - mem(dom2+DOM_PRESS)
    per_fac = c_extra(cp,FLOW_PERM)
    fnorm = c_nforce(cp)
    aper0 = c_extra(cp,FLOW_AP_ZERO)
    ; if fnorm > 0.0
    ;  aper = aper0-CC*fnorm/n_stiff ;* Fap_zero / (fnorm + Fap_zero)
    ;else
    ; if gap_mul = 0.0
    ;  aper = aper0
    ;else
    xdiff = b_x(b1) - b_x(b2)
ydiff = b_y(b1) - b_y(b2)
gap = sqrt(xdiff*xdiff+ydiff*ydiff) - b_rad(b1) - b_rad(b2)
    aper = aper0 + gap_mul * gap
  endif
  qpipe = pdiff * per_fac * aper^4 / rsum
dvol = qpipe * flow_dt
if xx1<0
if xx2>0
if yy1>x_min
if yy2<x_max
; xxx=xx2-xx1
; yyy=yy1-yy2
q_tot1=q_tot1+qpipe
end_if
end_if
end_if
end_if

if xx1<x_min/3
if xx2>x_min/3
if yy1 > x_min
if yy2 > x_max
xxx = xx2 - xx1
yyy = yy1 - yy2
q_tot2 = q_tot2 + qpipe;
end_if
end_if
end_if
if xx1 < x_max/3
if xx2 > x_max/3
if yy1 > x_min
if yy2 < x_max
xxx = xx2 - xx1
yyy = yy1 - yy2
q_tot3 = q_tot3 + qpipe;
end_if
end_if
end_if
end_if
q_tot4 = (q_tot1 + q_tot2 + q_tot3)/3
mem(dom1 + DOM_VSUM) = mem(dom1 + DOM_VSUM) - dvol
mem(dom2 + DOM_VSUM) = mem(dom2 + DOM_VSUM) + dvol
endif

cp = c_next(cp)
endLoop

;--- Pressure-changes in domains ...
dom = dom_head
loop while dom # null
if dom # outer_domain
if mem(dom + DOM_FIX) = 0
set_dom_coords
kk = mem(dom + DOM_BALL_LIST)
xd = 0.0
yd = 0.0
area_dom = 0.0
count = 0
loop while kk # null
bp = mem(kk+1)
xd = xd + abs(b_x(bp) - mem(dom + DOM_X))
yd = yd + abs(b_y(bp) - mem(dom + DOM_Y))
count = count + 1
kk = mem(kk)
endloop
area_dom = 0.5*(xd*xd + yd*yd)*lo_rad / count
delta_p = mem(dom+DOM_VSUM) * bulk_w / area_dom;
mem(dom+DOM_PRESS) = mem(dom+DOM_PRESS) + delta_p
endif
endif
mem(dom+DOM_VSUM) = 0.0
dom = mem(dom)
endLoop

;--- Pressure forces on balls ---
bp = ball_head
loop while bp # null
  b_xfap(bp) = 0.0
  b_yfap(bp) = 0.0
  bp = b_next(bp)
endloop
dom = dom_head
loop while dom # null
  if dom # outer_domain
    ppp = mem(dom+DOM_PRESS)
iadd = mem(dom+DOM_BALL_LIST)
bstart = mem(iadd+1)
loop while iadd # null
    next = mem(iadd)
    Abp = mem(iadd+1)
    if next = null
      Bbp = bstart
    else
      Bbp = mem(next+1)
    endif
    Arad = b_rad(Abp)
    Brad = b_rad(Bbp)
dpr = ppp / (Arad + Brad)
f1 = (b_y(Abp) - b_y(Bbp)) * dpr
f2 = (b_x(Bbp) - b_x(Abp)) * dpr
b_xfap(Abp) = b_xfap(Abp) + f1 * Arad
b_yfap(Abp) = b_yfap(Abp) + f2 * Arad
b_xfap(Bbp) = b_xfap(Bbp) + f1 * Brad
b_yfap(Bbp) = b_yfap(Bbp) + f2 * Brad
  iadd = next
  endif
endloop
endif
dom = mem(dom)
endLoop
end

def flow_bc ; Set flow-calc boundary conditions
; Range specified with (x1_bc .. x2_bc) and (y1_bc .. y2_bc)
; flow_set:  1  .. fix pressure
;            2  .. free pressure
;            3  .. set pressure to p_given
dom = dom_head
loop while dom # null
  if dom # outer_domain
    set_dom_coords
    xdom = mem(dom+DOM_X)
ydom = mem(dom+DOM_Y)
  endif
x6 = x_max + w_x(wadd6)
x8 = x_min + w_x(wadd8)

if ini = 1
  press_lin = P_pore
else
  press_lin = P_pore + p_given*(x6-xdom)/(x6-x8)
end if

if xdom > x1_bc
  if xdom < x2_bc
    if ydom > y1_bc
      if ydom < y2_bc
        caseOf flow_set
          case 1
            mem(dom+DOM_FIX) = press_lin ; 1
          case 2
            mem(dom+DOM_FIX) = press_lin; 0
          case 3
            mem(dom+DOM_PRESS) = press_lin; p_given
        endCase
      ; endif
    ; endif
  ; endif
endif
endif
endif
endif
endLoop
end

set echo on
flow_run
save dom1_perm.sav

---

**Permeability Estimation and Flow Input File:**

; FILE NAME: perm.data
new
set echo on
call dom_perm.data
call dom1_permx.data
;crk_init

plo crea _pres
plo add ball white white
plo add fish pressure green
;plo add fish crk_item blue red
;plo add cforce black yell
;plo add vel blue

131
plo add wall
plo sho
def pres_pos
wall_addr
zx11=x_min + w_x(wadd8)-x_max/10
zx12=x_min + w_x(wadd8)+x_max/10
zx21=x_max + w_x(wadd6)-x_max/10
zx22=x_max + w_x(wadd6)+x_max/10
zy1=y_min + w_y(wadd5)-x_max/10
zy2=y_max + w_y(wadd7)+x_max/10
end
pres_pos
;iterate
set gap_mul=1.0
;set CC=2.0
set bulk_w=2.2e9
def flood_exp
Press=1.0e3
visc=0.001
perm=3/(8*pi*visc)
ap_zero=3*lo_rad/20
flow_dr=0.001*2*0.4*lo_rad^4/(3*bulk_w*perm*ap_zero^4)
Area_flow=0.5*(lo_rad+hi_rad)*new_height
perm_value1=1.0e12*q_tot2*visc*2*(zx22-zx12)/(Area_flow*Press)
perm_value2=1.0e12*q_tot1*visc*2*(zx22-zx12)/(Area_flow*Press)
perm_value3=1.0e12*q_tot3*visc*2*(zx22-zx12)/(Area_flow*Press)
perm_value=0.5*(perm_value1+perm_value3)
kk=perm_value
perm_value4=1.0e12*abs(q_tot4)*visc*2*(zx22-zx12)/(Area_flow*Press)
q1=q_tot2
q2=q_tot1
q3=q_tot3
end
flood_exp
flow_props
set flow_set=1 ;x1_bc=zx11 x2_bc=zx12 y1_bc=zy1 y2_bc=zy2
flow_bc ; Left-hand fix condition
set flow_set=3 p_given=Press P_Pore=0.0e6 ; (NOTE: change to 2e5 for second case)
flow_bc ; Left-hand pressure
set flow_set=1 ini 1 ;x1_bc=zx21 x2_bc=zx22
flow_bc ; Right-hand fix condition (default pressure=0)
cyc 100
set ini 2
def prof ; Profile of pressure ... in x direction
loop n (1,nslice)
ytable(1,n) = 0 ; accumulates count
ytable(nsnap,n) = 0.0 ; accumulates pressure
endLoop
xmax = -1e20
xmin = 1e20
dom = dom_head
loop while dom # null
if dom # outer_domain
xmin = min(xmin,mem(dom+DOM_X))
xmax = max(xmax,mem(dom+DOM_X))
endif
dom = mem(dom+DOM_LINK)
endLoop
xdif = xmax - xmin
xinc = xdif / nslice
dom = dom_head
loop while dom # null
if dom # outer_domain
xx = mem(dom+DOM_X)
n = int((xx - xmin)/xinc) + 1
n = min(nslice,max(1,n))
xbar = (2*n-1)*xinc / 2.0 + xmin
ppp = mem(dom+DOM_PRESS)
xtable(nsnap,n) = xbar
ytable(nsnap,n) = ytable(nsnap,n) + ppp
ytable(1,n) = ytable(1,n) + 1
endif
dom = mem(dom+DOM_LINK)
endLoop
loop n (1,nslice)
    vvv= ytable(1,n)
ytable(nsnap,n) = ytable(nsnap,n) / ytable(1,n)
endLoop
def setTime
flood_exp
set hist_rep 1
hist id 188 perm_value1 flood_exp
hist id 177 perm_value flood_exp
hist id 199 perm_value3 flood_exp
hist id 201 perm_value4 flood_exp
hist id 101 q1 flood_exp
hist id 102 q2 flood_exp
hist id 103 q3 flood_exp
plot create Permeability_in_Darcy
plot hist 177 188 199
plot show
;plot create Flow_Rates
;plot hist 102 ;102 103
;plot sho
set nsnap=2
set nslice=25
cycle 50
prof
plot create _Profile
plot table nsnap
plot show
def setTime
oldtime = clock
end
def getTime
getTime = float(clock-oldTime)/100.0
end ;setTime

;print getTime
;END FILE: perm.data

Fish Subroutines File:

; Filename: fishcall.FIS
;
; PURPOSE: Defines the FISHcall macros for both PFC2D and PFC3D.
;
; Itasca Consulting Group, Inc.
;
;----------------------------------- FISHCALL DEFINITIONS ----------------
macro FC_CYC_MOT  0
macro FC_CYC_XMOT  1
macro FC_CYC_FORD  2
macro FC_CYC_XFORD 3
macro FC_BALL_CREATE 4
macro FC_BALL_DEL  5
macro FC_CONT_CREATE 6
macro FC_CONT_DEL  7
macro FC_BOND_CREATE 8
macro FC_BOND_DEL  9
macro FC_PB_CREATE 10
macro FC_PB_DEL 11
macro FC_CYC_TOP 12
; END OF Filename: fishcall.FIS

Crack Tracking File:

; Filename: crk.FIS
;
; PURPOSE: Crack tracking package for both PFC2D and PFC3D.

; FILES:
;    crk.FIS

; PACKAGE PREFIX: crk
;    Public functions and variables are intended to be utilized
;    and set by a package user, while private functions and
;    variables are utilized within the package itself, and in
;    general, should not be used or set by the package user.
;    All public functions and variables begin with the package
;    prefix; all private functions and variables begin with an
;    underscore.

; The following notation is employed within the package.
; All FISH variables and function names are enclosed by the
; set of brackets "[]". Occasionally, primary output
; variables of a FISH function are enclosed by the set of
; brackets "{}" immediately following the function call
; (e.g., "ss_cursr ; {ss_cstr(1...6)}" means that the six
; components of the array [ss_cstr] are set by the FISH
; function [ss_cursr]).

; PACKAGE USE:
;     1) When ready for crack tracking to begin, execute [crk_init].
;        All subsequent bond breakages will be tracked as cracks.
;     2) At any later point, use [crk_num*] variables to determine
;        number of cracks, and use [crk_item] and [crk_makeview] to
;        display the cracks.
;     3) The package can be reset at any time by calling [crk_init]
;        again. In this case, any current crack information will
;        be lost; and all subsequent bond breakages will be tracked
;        as cracks.

; HISTORY: created    David Potyondy  27-Jul-95
;           last mod.  DOP  05-Dec-95
;           last mod.  DOP  25-Jan-96 (made [crk_init] re-entrant)
;           last mod.  DOP  02-Feb-96 (crk plotting uses mark-fields)
;           last mod.  DOP  12-Feb-96 (crk plotting active for 3D)

; TRACKING CRACK FORMATION
;    Cracks may only form between initially bonded particles. Each
;    crack has a datablock associated with it. All datablocks are stored
;    in a linked list whose header is [crk_head]. When a bond breaks, a
;    datablock is created and added to the list. The current mechanism
;    assumes that there is either a contact bond or a parallel bond present
;    initially, not both.
;    The contents of each crack-datablock follow:
(0 - crk_NEXT) - ptr. to next datablock in llist
(1 - crk_MARK) - integer field used during traversals
(2 - crk_BALL1) - ptr. to parent ball-1
(3 - crk_BALL2) - ptr. to parent ball-2
(4 - crk_FAIL) - integer bond failure indicator
   Assumes only one type of bond initially present.
   (0=not set; 1=contact bond failed normal;
    2=contact bond failed shear;
    3=parallel bond failed normal;
    4=parallel bond failed shear)
(5 - crk_TM) - float time of failure (time since call crk_init())
(6 - crk_CYC) - integer cycle number at failure

Global variables (public):
   crk_head - head of llist of crack datablocks
   crk_tail - tail of llist of crack datablocks
   crk_time0 - problem time when crk-package was initialized
   crk_num - total # of cracks
   crk_num_cnf - total # contact bond failures in normal mode
   crk_num_csf - total # contact bond failures in shear mode
   crk_num_pnf - total # parallel bond failures in normal mode
   crk_num_psf - total # parallel bond failures in shear mode
   crk_radmult - crack radius multiplier

Related Functions (public) (in/out vars. designated by {}):
   crk_init
   _crk_init
   _crk_getdata
   crk_chk_crkdata
   crk_time_bounds
   crk_fil_reset
   crk_fil_all
   _crk_fil_cyc_interval {crk_fil_cyc_min, crk_fil_cyc_max}
   _crk_item {crk_icon, crk_iconmult, crk_ctype}
   crk_makeview
   crk_destroyview

Related Functions (private):
   _crk_newblock
   _crk_formcb
   _crk_formpb
   _crk_num_mark
   _crk_b_add
   _crk_chk_crack

PUBLIC FUNCTIONS
==================================================================

def crk_init
   
   ---- Initialize the crack tracking mechanism. All subsequent bond
   breaks will be stored as a crack formation event.
This function is re-entrant --- i.e., if the package has already been initialized, all subsequent calls result in deletion of existing crack-data and reinitialization.

OUTPUT: crk_head - head of list of crack datablocks
        crk_tail - last block in list of crack datablocks
        crk_num... - global crack number counters
        crk_time0 - problem time when crk-package was initialized
        crk_radmult - crack radius multiplier

if _crk_reentrant = 1 then ; will be zero upon first entrance
  _crk_destroyllist
else
  _crk_reentrant = 1
command
  set fishcall FC_BOND_DEL _crk_formcb
  set fishcall FC_PB_DEL _crk_formpb
end_command

; --- Define crack datablock entry offsets
crk_NEXT   = 0
crk_MARK   = 1
crk_BALL1  = 2
crk_BALL2  = 3
crk_FAIL   = 4
crk_TM     = 5
crk_CYC    = 6
crk_NUMDB  = 7  ; # entries in datablock
end_if

; --- Initialize global crack-related variables
crk_head = null
crk_tail = null
crk_time0 = time
crk_radmult = 1.0  ; default value, reset after calling crk_init()
crk_num = 0
 crk_num_cnf = 0
 crk_num_csf = 0
 crk_num_pnf = 0
 crk_num_psf = 0
end

----------------------------------------------------------------------------------------------------------------------------------
def crk_getdata

; ----- Computes crack data for [crkp] datablock.
; Each crack is assumed to be a cylinder. The thickness equals the gap between the two parent particles. The radius is given by the intersection of the cylinder bisection plane with a membrane stretched tightly between the two parent particles. The centroid lies along the line between the centers of the two parent particles and bisects the gap between the two
; parent particles.

; INPUT:  crkp - pointer to crack datablock
;        crk_radmult - crack radius multiplier
; OUTPUT: _crk_fail - integer failure type (see crk_FAIL in datablock)
;         _crk_ball1 - pointer to parent ball-1
;         _crk_ball2 - pointer to parent ball-2
;         _crk_x    - x-coordinate of crack centroid
;         _crk_y    - y-coordinate of crack centroid
;         _crk_z    - z_coordinate of crack centroid (if dim=3)
;         _crk_gap  - aperture of crack (thickness of cylinder)
;         _crk_rad  - crack radius (adjusted by crk_radmult)
;         _crk_normx - x_component of crack unit-normal (ball1 to ball2)
;         _crk_normy - y_component of crack unit-normal (ball1 to ball2)
;         _crk_normz - z_component of crack unit-normal (ball1 to ball2)
;               (if dim=3)
;         _crk_time - time when crack formed
;               (elapsed time since call to (crk_init()))
;         _crk_cycle - cycle number when crack formed
; LOCAL:  vec12x, vec12y, vec12z - vector from ball1 to ball2
;       bR1, bR2 - radii of balls 1 and 2
;       dist - distance between ball centers

; _crk_ball1 = mem(crkp+crk_BALL1)
; _crk_ball2 = mem(crkp+crk_BALL2)

bR1 = b_rad(_crk_ball1)
bR2 = b_rad(_crk_ball2)

vec12x = b_x(_crk_ball2) - b_x(_crk_ball1)
vec12y = b_y(_crk_ball2) - b_y(_crk_ball1)

case_of dim
  case 2:
    dist = sqrt( vec12x*vec12x + vec12y*vec12y )
    _crk_normx = vec12x / dist
    _crk_normy = vec12y / dist
  case 3:
    vec12z = b_z(_crk_ball2) - b_z(_crk_ball1)
    dist = sqrt( vec12x*vec12x + vec12y*vec12y + vec12z*vec12z )
    _crk_normx = vec12x / dist
    _crk_normy = vec12y / dist
    _crk_normz = vec12z / dist
end_case

_crk_gap = dist - bR1 - bR2

mult = bR1 + (_crk_gap / 2.0)
_crk_x = b_x(_crk_ball1) + mult * _crk_normx
_crk_y = b_y(_crk_ball1) + mult * _crk_normy
if dim = 3 then
  _crk_z = b_z(_crk_ball1) + mult * _crk_normz
end_
_crk_rad = bR1 + (bR2 - bR1) * (mult / dist)
_mcrk_rad = crk_radmult * _crk_rad

end
; def crk_chck_crkdata
;
; ----- Dumps crack datablock for crack (if it exists) between two
;       given balls.
;
; INPUT: crk_chck_bid1, crk_chck_bid2 - parent balls of potential crack
;
_; crk_chck_bid = crk_chck_bid1
; crk_chck_ball1 = _crk_b_add
_; crk_chck_bid = crk_chck_bid2
; crk_chck_ball2 = _crk_b_add
;if _crk_chck_crack = 0 then
; _txtstr = "'
; _txtstr = _txtstr + 'No crack between balls '+string(crk_chck_bid1)
; _txtstr = _txtstr + ' and '+string(crk_chck_bid2)
; ii = out( _txtstr )
; exit
else
; _txtstr = "'
; _txtstr = _txtstr + 'Data for crack between balls '+string(crk_chck_bid1)
; _txtstr = _txtstr + ' and '+string(crk_chck_bid2)+' follows. . .'
; ii = out( _txtstr )
end_if

; crkp = _crk_chck_crkp
; crk_getdata
; ii = out(''_crk_x = '+string(_crk_x))
; ii = out(''_crk_y = '+string(_crk_y))
; ii = out(''_crk_z = '+string(_crk_z))
; ii = out(''_crk_mark = '+string(_crk_mark))
; ii = out(''_crk_fail = '+string(_crk_fail))
; ii = out(''_crk_gap = '+string(_crk_gap))
; ii = out(''_crk_rad = '+string(_crk_rad))
; ii = out(''_crk_normx = '+string(_crk_normx))
; ii = out(''_crk_normy = '+string(_crk_normy))
; ii = out(''_crk_normz = '+string(_crk_normz))
; ii = out(''_crk_time = '+string(_crk_time))
; ii = out(''_crk_cycle = '+string(_crk_cycle))
end
;==================================================================
def crk_time_bounds
;

139
; ----- Determine min./max times stored in all cracks with mark-field
; set to 1.
;
; INPUT: crk_head
; OUTPUT: crk_mintime, crk_maxtime
;
crk_mintime = 1e20
crk_maxtime = 0.0
crkp = crk_head
loop while crkp # null
  crk_getdata
  if _crk_mark = 1 then
    if _crk_time > crk_maxtime then
      crk_maxtime = _crk_time
    end_if
    if _crk_time < crk_mintime then
      crk_mintime = _crk_time
    end_if
  end_if
  crkp = mem(crkp+crk_NEXT)
end_loop
end

;==================================================================
def crk_item
;
; ----- Generates a plotitem for visualizing the set of cracks in
; the model. The input parameters to this function control
; the visualization mapping. Only cracks with their mark-
; fields set to 1 are plotted. Mark-fields are set via
; filter functions: [crk_fil_xxx].
; The plotitem is activated by typing: PLOT ADD CRK_ITEM
;
; Visualization Mapping
;
; Two types of crack icons are supported for both 2D and 3D.
; For 2D:
;    If [crk_icon=0], each crack is drawn as a straight line of
;    length [crk_len] centered at the crack location and
;    perpendicular to [crk_norm]. If [crk_icon=1], then each
;    crack is drawn as a solid circle of diameter [crk_len] and
;    centered at the crack location.
; For 3D:
;    If [crk_icon=0], each crack is drawn as a 8-sided polygon
;    inscribed in circle of radius [crk_rad] and centered at
;    crack centroid and perpendicular to [crk_norm].
;    If [crk_icon=1], each crack is drawn as a sphere centered
;    at crack centroid.
;
; The color of each icon indicates either bond failure type or
; time of failure. If [crk CType=0] then color index of each
; icon is set in the range [1,4] such that:
; 1-contact bond normal failure; 2-contact bond shear failure;
; 3-parallel bond normal failure; 4-parallel bond shear failure.
; If [crk_ctype=1] then color index of each icon is set in the
; range [1,16] (green to red) to indicate the time of crack
; formation (early is green, late is red).
;
; INPUT:  crk_head   - head of list of crack datablocks
;         crk_icon   - display icon
;              (if =0, lines; if =1, filled circles)
;         crk_iconmult - multiplier for size of icons
;              (if =0.0, defaults to 1.0)
;         crk_ctype  - color mapping for icon
;              (if =0, failure type; if =1, failure time)
;
; Define arrays used by [crk_draw...] functions.
plot_item
Array _crk_pt1(dim)
Array _crk_pt2(dim)
Array _crk_poly(dim,8)

if crk_iconmult = 0.0 then
  crk_iconmult = 1.0
end_if

if crk_ctype = 1 then
  _plt_numcon = 16
  crk_time_bounds
  _plt_incr = (crk_maxtime - crk_mintime) / _plt_numcon
end_if

stat=set_line_width(1)  ; for 2D, and [crk_icon]=0

crkp = crk_head
loop while crkp # null
  crk_getdata
  if _crk_mark = 1 then
    case_of crk_ctype
    case 0 ; color based on failure type
      _cindex = _crk_fail - 1
    case 1 ; color based on time of failure
      if _plt_incr = 0.0 then
        _cindex = 0
      else
        _cindex = int( (_crk_time - crk_mintime) / _plt_incr )
      end_if
    end_case
    stat = set_color( _cindex )
  end_case

  case_of crk_icon
  case 0 ; lines (2D) / near-circular polygons (3D)
  case_of dim
    case 2
stat = _crk_draw2d_line
case 3
  stat = _crk_draw3d_polygon
end_case
case 1 ; filled circles (2D) / filled spheres (3D)
case_of dim
case 2
  stat = _crk_draw2d_circle
case 3
  stat = _crk_draw3d_sphere
end_case
end_case
end_if ; mark-field set to 1

if stat = -1 then ; terminate plot
  exit
end_if

crkp = mem(crkp+crk_NEXT)
end_loop
end

; ===================================================================
def crk_fil_reset
;
; ----- Crack-display filter. Sets mark field to 0 for all cracks.
;
  crkp = crk_head
loop while crkp # null
    mem(crkp+crk_MARK) = int(0)
  crkp = mem(crkp+crk_NEXT)
end_loop
end

; ===================================================================
def crk_fil_all
;
; ----- Crack-display filter. Sets mark field to 1 for all cracks.
;
  crkp = crk_head
loop while crkp # null
    mem(crkp+crk_MARK) = int(1)
  crkp = mem(crkp+crk_NEXT)
end_loop
end

; ===================================================================
def crk_fil_cyc_interval
;
; ----- Crack-display filter. Sets mark field to 1 for all cracks
; that were formed (inclusively) btn. cycles [crk_fil_cyc_min]
; and [crk_fil_cyc_max].
;
; INPUT: crk_fil_cyc_min, crk_fil_cyc_max
;
crkp = crk_head
loop while crkp # null
    crk_getdata
    _hit = 0
    if _crk_cycle >= crk_fil_cyc_min then
        if _crk_cycle <= crk_fil_cyc_max then
            _hit = 1
        end_if
    end_if
    if _hit = 1 then
        mem(crkp+crk_MARK) = int(1)
    end_if
    crkp = mem(crkp+crk_NEXT)
end_loop
end

--- Creates a plot-view called "view_of_cracks" that contains the
[crk_item] plotitem with text and colors set to current values
of the crack plotting parameters ([crk_icon], [crk_iconmult],
[crk_ctype]). If the settings are changed, [crk_makeview] should
be called again: it will update itself.

NOTE: Do not destroy this view manually, rather use [crk_destroyview].

INPUT: crk_ctype, crk_icon, crk_iconmult (see [crk_item] for descrip.)

if crk_iconmult = 0.0 then
    crk_iconmult = 1.0
end_if
if _crk_viewexists = 1 then
    crk_destroyview
end_if

_txtstr = 'micro-cracks (' + string(_crk_num_mark) + ')
command
    plot create view_of_cracks
    plot add crk_item
    plot mod 1 alias _txtstr
    plot cur view_of_cracks
end_command

_case_of crk_ctype
    case 0
        macro '_plt_spectrum' 'yellow black yellow black'
end_command
case_of crk_icon
  case 0
    case_of dim
      case 2
        _txtstr = 'Cracks (lines): '
      case 3
        _txtstr = 'Cracks (polygons): '
    end_case
  case 1
    case_of dim
      case 2
        _txtstr = 'Cracks (circles): '
      case 3
        _txtstr = 'Cracks (spheres): '
    end_case
    _txtstr = _txtstr + '[yellow/black]=normal/shear fail '
  case 1
    _plt_numcon = 16
    _plt_init ; {_plt_spectrum}
    _txtstr = 'Micro-cracks: '
    _txtstr = _txtstr + '16 grays [light/dark]=early/late]
  end_case
  _txtstr = _txtstr + '(mag='+string(crk_iconmult)+')'
command
  plot mod 1 _plt_spectrum
  plot set title text _txtstr
end_command
end
;
; def crk_destroyview
; ; ----- Destroys the plot-view created by [crk_makeview].
; if _crk_viewexists = 1 then
  command
    plot cur 0
    plot destroy view_of_cracks
  end_command
end_if
  _crk_viewexists = 0
end
;
def _crk_newblock
; ; ----- Creates and initializes a new crack datablock and adds it
to end of llist.
; OUTPUT: crkp - pointer to the new block
; EFFECT: crk_head, crk_tail
;
crkp = get_mem(crk_NUMDB)

; --- Initialize datablock entries
mem(crkp+crk_NEXT) = null
mem(crkp+crk_MARK) = int(1)
mem(crkp+crk BALL1) = null
mem(crkp+crk BALL2) = null
mem(crkp+crk_FAIL) = int(0)
mem(crkp+crk_TM) = float(0.0)
mem(crkp+crk_CYC) = int(0)

if crk_head = null then
  crk_head = crkp
  crk_tail = crkp
else
  mem(crk_tail+crk_NEXT) = crkp
  crk_tail = crkp
end_if
end

def _crk_destroyllist
;
; ----- Destroy entire llist of crack datablocks and free the memory.
;
; INPUT: crk_head
;
i = out('[_crk_destroyllist]: Destroying all crack datablocks.]
  crkp = crk_head
loop while crkp # null
  crkp = mem(crkp+crk_NEXT)
  kk = lose_mem(crk_NUMDB, crkp)
  crkp = crkp
end_loop
end

def _crk_formcb
;
; ----- Form crack as result of contact bond breakage.
; Create crack datablock.
; (Register via "set fishcall FC_BOND_DEL _crk_formcb").
;
; cp = fc_arg(0)
failmode = fc_arg(1)

  _crk_newblock
mem(crkp+crk BALL1) = c_ball1(cp)
mem(crkp+crk BALL2) = c_ball2(cp)
crk_num = crk_num + 1
if failmode = 0 then ; normal failure
    mem(crkp+crk_FAIL) = 1
    crk_num cnf = crk_num cnf + 1
end_if
if failmode = 1 then ; shear failure
    mem(crkp+crk_FAIL) = 2
    crk_num csf = crk_num csf + 1
end_if
mem(crkp+crk_TM) = float( time - crk_time0 )
mem(crkp+crk_CYC) = int( step )
end

def _crk_formpb
    ; ----- Form crack as result of parallel bond breakage.
    ;       Create crack datablock.
    ;       (Register via "set fishcall FC_PB_DEL _crk_formpb").
    ;
    cp = fc_arg(0)
    failmode = fc_arg(1)

    _crk_newblock
    mem(crkp+crk_BALL1) = c_ball1(cp)
    mem(crkp+crk_BALL2) = c_ball2(cp)

    crk_num = crk_num + 1
    if failmode = 0 then ; normal failure
        mem(crkp+crk_FAIL) = 3
        crk_num_pnf = crk_num_pnf + 1
    end_if
    if failmode = 1 then ; shear failure
        mem(crkp+crk_FAIL) = 4
        crk_num_psf = crk_num_psf + 1
    end_if

    mem(crkp+crk_TM) = float( time - crk_time0 )
    mem(crkp+crk_CYC) = int( step )
end
def _crk_num_mark
    ; ----- Returns number of cracks with their mark-fields set to 1.
    ;
    _crk_num_mark_ = 0
    crkp = crk_head
    loop while crkp # null
        crk_getdata
        if _crk_mark = 1 then
            _crk_num_mark_ = _crk_num_mark_ + 1
        end_if
        crkp = mem(crkp+crk_NEXT)
    end_loop
    _crk_num_mark = _crk_num_mark_
end

def _crk_b_add
    ; ----- Returns pointer to given ball. If ball does not exist,
    ;       returns null-pointer.
    ;
    ; INPUT: _crk_bid - id number of ball
    ;
    _crk_b_add = null
    bp = ball_head
    loop while bp # null
        if b_id(bp) = _crk_bid then
            _crk_b_add = bp
            exit
        endif
        bp = b_next(bp)
    end_loop
end

def _crk_chk_crack
    ; ----- Returns (1) if a crack exists between the two given balls;
    ;       else returns (0). Also, returns crack-pointer if crack exists.
    ;
    ; INPUT: crk_chk_ball1, crk_chk_ball2 - ptrs. to balls to check
    ;
    ; OUTPUT: _crk_chk_crkp - crack-pointer
    ;
    exist = 0
    section
        crkp = crk_head
        loop while crkp # null
            crk_getdata
            if _crk_ball1 = crk_chk_ball1 then
                if _crk_ball2 = crk_chk_ball2 then
                    exist = 1
                    exit section
                endif
            endif
            crkp = mem(crkp+crk_NEXT)
        end_loop
    end_section

    _crk_chk_crkp = crkp
    _crk_chk_crack = exist
def _plt_init
;
; ----- Initialize the spectrum of colors for given number of contour
;       intervals [_plt_numcon]. Current spectrum is for GREEN-RED.
;
; INPUT: _plt_numcon - number of contour intervals
;
; OUTPUT: _plt_spectrum - macro of [_plt_numcon] colors to be
;     used as: "plot add ball _plt_spectrum"
;
num_col = _plt_numcon - 1
all_col = ' '
loop nn (0,num_col)
  mcol = 'c'+ string(nn)
  rat  = 0.95*(1.0 - float(nn) / float(num_col))
  ggg = 'gray '+string(rat)
  command
    macro mcol ggg
  end_command
  all_col = all_col + mcol + ' '
end_loop
command
  macro '_plt_spectrum' all_col
end_command
end

def _crk_draw2d_line
;
; ----- Draws 2D crack as a straight line of length [_crk_len]
;       centered at the crack location and perpendicular to
;       Returns status of draw command.
;
; INPUT: crk_getdata - has been called for this crack
 ;       crk_iconmult
 ;
 _crk_pt1(1) = _crk_x - crk_iconmult*_crk_rad * _crk_normy
 _crk_pt1(2) = _crk_y + crk_iconmult*_crk_rad * _crk_normx
 _crk_pt2(1) = _crk_x + crk_iconmult*_crk_rad * _crk_normy
 _crk_pt2(2) = _crk_y - crk_iconmult*_crk_rad * _crk_normx

 _crk_draw2d_line = draw_line( _crk_pt1, _crk_pt2 )
end

def _crk_draw2d_circle
;
; ----- Draws 2D crack as a solid circle of diameter [_crk_len]
;       and centered at the crack location.
;       Returns status of draw command.
;
; INPUT: crk_getdata - has been called for this crack
 ;       crk_iconmult
 ;
 _crk_pt1(1) = _crk_x
 _crk_pt1(2) = _crk_y
 _rad = crk_iconmult * _crk_rad
_crk_draw2d_circle = fill_circle( _crk_pt1, _rad )
end

def _crk_draw3d_polygon
;
; ----- Draws 3D crack as a 8-sided polygon inscribed in circle
; of radius [_crk_rad] and centered at crack centroid and
; perpendicular to [_crk_norm].
; Returns status of draw command.
;
; INPUT: crk_getdata - has been called for this crack
; crk_iconmult
;
zero_tol = 1e-6

nx = _crk_normx
ny = _crk_normy
nz = _crk_normz
n_parallel = 0
if abs(nx - ny) < zero_tol then
  if abs(nx - nz) < zero_tol then ; n = alpha*(1,1,1)
    n_parallel = 1
    tx = 1.0
    ty = -1.0
    tz = 0.0
  end_if
end_if
if n_parallel = 0 then
  tx = ny - nz
  ty = nz - nx
  tz = nx - ny
end_if
dist = sqrt(tx*tx + ty*ty + tz*tz)
  tx = tx / dist
  ty = ty / dist
  tz = tz / dist
  sx = ny*tz - nz*ty
  sy = nz*tx - nx*ty
  sz = nx*tx - ny*tz
  vx = tx + sx
  vy = ty + sy
  vz = tz + sz
  dist = sqrt(vx*vx + vy*vy + vz*vz)
  vx = vx / dist
  vy = vy / dist
  vz = vz / dist
  wx = tx + sx
  wy = ty + sy
  wz = tz + sz
  dist = sqrt(wx*wx + wy*wy + wz*wz)
  wx = wx / dist
  wy = wy / dist
  wz = wz / dist

_rad = crk_iconmult * _crk_rad
_crk_poly(1,1) = _crk_x + _rad * _tx
_crk_poly(2,1) = _crk_y + _rad * _ty
_crk_poly(3,1) = _crk_z + _rad * _tz
_crk_poly(1,2) = _crk_x + _rad * _vx
_crk_poly(2,2) = _crk_y + _rad * _vy
_crk_poly(3,2) = _crk_z + _rad * _vz
_crk_poly(1,3) = _crk_x + _rad * _sx
_crk_poly(2,3) = _crk_y + _rad * _sy
_crk_poly(3,3) = _crk_z + _rad * _sz
_crk_poly(1,4) = _crk_x - _rad * _wx
_crk_poly(2,4) = _crk_y - _rad * _wy
_crk_poly(3,4) = _crk_z - _rad * _wz
_crk_poly(1,5) = _crk_x - _rad * _tx
_crk_poly(2,5) = _crk_y - _rad * _ty
_crk_poly(3,5) = _crk_z - _rad * _tz
_crk_poly(1,6) = _crk_x - _rad * _vx
_crk_poly(2,6) = _crk_y - _rad * _vy
_crk_poly(3,6) = _crk_z - _rad * _vz
_crk_poly(1,7) = _crk_x - _rad * _sx
_crk_poly(2,7) = _crk_y - _rad * _sy
_crk_poly(3,7) = _crk_z - _rad * _sz
_crk_poly(1,8) = _crk_x - _rad * _wx
_crk_poly(2,8) = _crk_y - _rad * _wy
_crk_poly(3,8) = _crk_z - _rad * _wz
_crk_draw3d_polygon = fill_poly( _crk_poly, 8 )
end

def _crk_draw3d_sphere
; ----- Draws 3D crack as a sphere centered at crack centroid.
;       Returns status of draw command.
;
; INPUT: crk_getdata - has been called for this crack
;       crk_iconmult
;       _crk_iconmult
;       _crk_pt1(1) = _crk_x
;       _crk_pt1(2) = _crk_y
;       _crk_pt1(3) = _crk_z
;       _rad = crk_iconmult * _crk_rad
;       _crk_draw3d_sphere = fill_circle( _crk_pt1, _rad )
end

return
; END OF Filename: crk.FIS