Hydraulic fracturing with distinct element method

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DEPARTMENT STRATEGIC RESEARCH
Project manager : ir. J.P. Pruiksma
Project supervisor : ir. A. Bezuijen

GeoDelft
Stieltjesweg 2, 2628 CK DELFT
Postbus 69, 2600 AB DELFT
The Netherlands

Telephone (+31) 15 - 269 35 00
Telefax (+31) 15 - 261 08 21
Postal account 234342
Bank MeesPierson NV
Account 25.92.35.911
In this report, hydraulic fracturing is investigated using the distinct element code PFC2D from Itasca. Special routines were written to be able to model hydraulic fracturing. These include adding fluid flow to PFC2D and updating the fluid flow domains when fractures appear. A brief description of this implementation and the modelling of the hydraulic fracturing is given.

After the set-up of the hydraulic fracturing simulations has been discussed, with all the main input parameters, several main parameters are varied to study the resulting fracture patterns, pressure distributions and borehole pressures. These parameter studies are: particle size dependency of the simulations, behaviour at various confining stresses, the influence of the internal friction angle of the sand and the fracturing behaviour for different borehole injection rates. After this parameter study, comparisons are made with experiments done at TU Delft, GeoDelft and in the literature. The simulation results show the same trends as the experiments and are also in good agreement quantitatively.
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1 Introduction

To gain insight in the hydraulic fracturing of loose sand, both experimental and numerical research has been done. One of the numerical methods chosen to model the hydraulic fracturing process is a two-dimensional distinct element method, where distinct particles are used to describe a sample with grain-like behaviour similar to that of sand. The used code is PFC2D from Itasca in which additional routines were programmed to be able to model hydraulic fracturing.

In a previous GeoDelft report, CO386730/05: “Biaxial test simulations with PFC2D”, a description of biaxial test simulations has been given that were performed to find the relation between distinct element particle parameters and macroscopic behaviour of the sample. Using these biaxial test simulations, a set of parameters for the distinct particles was found that model a material having the characteristics of Swedish Baskarp sand used in the fracturing experiments. The report on PFC2D biaxial test simulations is also included in this report as Appendix VII. These biaxial tests were done for dry sand, since the standard PFC2D code only works with dry assemblies of particles without any consideration of pore fluid. In another GeoDelft report, CO386730/11: “Fluid flow in PFC2D”, included here as appendix VIII, the implementation of pore fluid in PFC2D was discussed extensively. The standard PFC2D code for dry assemblies was extended with extra routines describing fluid flow. The interaction of flow with deformation of the borehole and fully coupled flow were also investigated.

In this report, the results of various hydraulic fracturing simulations are presented. The hydraulic fracturing simulations were made with a fully coupled borehole (full interaction between fluid and particles), but with the rest of the sample uncoupled due to the high computation times for fully coupled flow as described in Appendix VIII. Many parameters, like particle size, confining stress, injection rate and angle of internal friction, were varied to see their influence on the fracturing behaviour. The results of these fracturing simulations are compared with theory and fracturing experiments to assess the effectiveness of distinct elements in describing hydraulic fracturing and also to obtain insights into the fracturing process itself in order to give certain relationships between model parameters and the fracturing behaviour.

In Chapter two, a short overview of the standard PFC2D code and the implementation of fluid flow in PFC2D will be given. Chapter 3 discusses the parameters that will be used in the hydraulic fracturing simulations and Chapter 4 describes the set-up of hydraulic fracturing simulations. Chapters five to nine describe results for all the various hydraulic fracturing simulations that have been made for loose sand, where particle size, confining stress, injection rate and friction angle have been varied. Chapter ten compares the simulation results with various experiments done at TU Delft and GeoDelft as well as experiments from the literature.
2 Implementation of hydraulic fracturing in PFC2D

The distinct element code PFC2D by Itasca is capable of describing the movement of particles in a particle assembly under influence of external forces and inter-particle forces in two dimensions. In this chapter, the general functioning of PFC2D is presented together with the addition of pore fluid in the code by use of the embedded FISH programming language. Also the set-up and various parameters of the hydraulic fracturing simulation are presented.

2.1 The standard PFC2D code

The PFC2D program is capable of describing the dynamic motion of an assembly of particles. Because the code is two-dimensional, particles are presented as 2D circles. These circles are set to have the mass and moment of inertia of discs of unit-thickness (although it’s also possible in PFC2D to let the particles have the mass and moment of inertia characteristics of a sphere). Particles in contact exert a normal and a shear force on each other. The normal force is determined by the distance the particles overlap with each other. The shear force is determined by the opposite rotation of two overlapping particles. The shear force can not be higher than a user given fraction of the normal force. This fraction is related to the friction angle and is called friction coefficient.

For each particle, the shear and normal forces acting upon it through contact with neighbouring particles and walls are summed to give the total force and moment acting on the particle. Because the code is two-dimensional, the total force has to components X and Y, and the total moment is in the out of plane direction (Z). With Newton’s second law and explicit time integration, the displacement of the particles (translation and rotation) in a time step is determined. The PFC2D code determines a stable time step which depends on the stiffness of the particles. After one time step and displacement, again the contact forces are calculated giving a new total force on each particle needed for the next step. The process continues for a number of time steps defined by the user or until a certain equilibrium criterion has been reached.

In the standard PFC2D code there are two contact constitutive models: a linear model and a non-linear Hertz-Mindlin model. Both models were used in the earlier biaxial test simulations, see Appendix VII. Detailed information about the contact models can be found in the PFC2D manual [Itasca].

2.2 Fluid flow and coupled borehole simulation

A detailed description of all aspects related to fluid flow in PFC2D is given in the fluid flow report included here as Appendix VIII. Here, only a brief overview of the method is presented.

2.2.1 Domain structure and flow laws

To model fluid flow, some kind of mesh has to be created within the assembly of particles. This mesh is formed by closed rings of particles that are in contact, see Figure 2.1. Such a ring is called a domain. The shape of the domains varies, as the number of particles in a ring varies. The borehole will be a ring of many particles and so will have many sides, while most domains in a general randomly closely packed assembly will be triangular in shape. The fluid pressure is the main variable and each domain has it’s own fluid pressure. The domain structure is updated when contacts break or are created during the deformation calculation and the pressure is also updated for the newly created
domains by either averaging in case of a merging of two domains or having the same value as the old
domain when one domain is split in two. It is assumed that fluid flows in or out of a domain through
the contacts between the particles, and that the flow rate is proportional to the pressure difference. In
this way, fluid flow is modelled as a network of connecting “tubes”, see Figure 2.1.

![Diagram of domain structure with labels for domain boundaries, flow domain connections, and flow domain centers.](image)

Figure 2.1: Domain structure used for fluid flow in PFC2D.

In the report on fluid flow (Appendix VIII), it has been shown that this implementation of fluid flow
best matches results of analytical Darcy flow when the flow rate $q_c$ through each contact is given by:

$$q_c = \sqrt{3} \frac{\kappa}{\mu} (p_{dom2} - p_{dom1})$$

(2.1)

Where $\kappa$ is the intrinsic permeability of the material and $\mu$ the viscosity of the fluid. By calculating $q_c$
for each contact in a domain, the sum equals the total flow rate into the domain. By choosing a

timestep $\Delta t$, the volume of fluid that flows into a domain can be calculated:

$$\Delta V = \Delta t \sum_i q_c^i$$

(2.2)

Here the sum is over all contacts in a domain. With the volume inflow, a pressure change can be
calculated:

$$\Delta p = K_f \frac{\Delta V}{V_{dom}}$$

(2.3)
Here $K_f$ is the fluid bulk modulus and $V_{\text{dom}}$ is the pore volume of the considered domain. This pore volume is calculated in the code by calculating the area of the polygon that makes up the domain and multiplying it by a user defined porosity. Calculating porosity as the void ratio inside the polygon, namely the total area of the polygon minus the area of the particles lying inside this polygon divided by the total polygon area, gives too low porosity values because of the 2D nature, see Appendix VIII.

2.2.2 Interaction of fluid with particles

Now fluid flow has been modelled, there must be an interaction with the particles in order to have an effect in the distinct element simulation. Suppose that a certain particle is part of four domains, as shown in Figure 2.2. Then in each of the domains surrounding the particle is a fluid pressure. These different pressures act on the particle. In the code the pressures are integrated over the part of the circle lying in the specified domain. This integration gives a contribution to the total force on the particle. The integration in each domain surrounding the particle is carried out and summed to give the total force by the fluid on the particle $F_{\text{fluid}}$.

![Figure 2.2: Fluid interaction with particles.](image)

It is also possible that a particle is contained within a domain, and is no part of the domain structure itself, see Figure 2.3. In this case the particle is surrounded with fluid having a constant pressure and the resulting net force due to fluid pressure that acts on the particle is zero. In a hydraulic fracturing simulation this is most likely to happen inside the borehole domain. In such situation a particle would bounce around inside the borehole due to the dynamic nature of the PFC2D code. To prevent this, it has been implemented that a Stokes force is acting on the particle. Namely, the particle is thought to be most influenced by the fluid flow through the nearest contact. Then the force on the particle is calculated from $F = 6\pi\mu R v$, where $\mu$ is the viscosity of the fluid, $R$ the particle radius and $v$ the speed of the fluid relative to the particle. If the flow is out of the domain where the particle is, as is the case for the borehole domain when fluid is injected during hydraulic fracturing, then this Stokes force will drive the particle to the domain wall and it will stay there, see also Figure 2.3. Especially during hydraulic fracturing it is likely to happen that particles in the borehole wall become loose due to the fluid infiltration and decreasing effective stress.
Figure 2.3: Example of a "loose" particle not being part of the domain structure but contained inside a domain, in this case the borehole domain. A Stokes force $F$ is acting on the particle calculated from the flow through the nearest contact.

For each particle the total force due to fluid pressure (or Stokes flow) is calculated and the X and Y components of this force are stored in the external force addresses for each particle. Now, the standard PFC2D code uses this external force, in addition to the inter-particle forces, for the computation of the displacements.

### 2.2.3 One-way coupled flow and fully coupled flow

Fluid pressure gives rise to an extra force on the particles, which in turn affects the movement of the particles. In a realistic simulation, movement of particles also causes deformation of the domains and a change in pore volume, giving rise to a change in pore pressure in turn affecting the movement of the particles together with the flow. This is called fully coupled flow and is discussed in more detail in Appendix VIII. Fully coupled flow was implemented but turned out to be computationally intensive as calculations took a long time to complete.

Therefore, the choice has been made to do the fracturing simulations with one-way coupling for all the domains except the borehole, which has been modelled as a fully coupled domain. In this way, injection controlled simulations can be made. Namely, when an injection rate is chosen, there is a certain constant flow rate into the borehole. The flow into the borehole minus the flow out of the borehole wall, gives rise to a pressure change of the borehole. If the borehole expands, because of an increase in pressure, the pressure drops now with expansion as expected because of fully coupling of the borehole. So for the borehole, the pressure is determined by the injection rate, the flow out of the domain and the volume change by expansion. The other domains only have fluid flow to control their pressure, but the pressure does affect the displacements as mentioned above. It’s just that for these domains the deformations itself don’t cause a pressure change.

### 2.3 Model generation and contact properties

The basic features of the PFC2D code and the implemented fluid flow and coupling have been discussed previously and here the generation of the model and particle assembly will be discussed. To create the sample in PFC2D, first a square area is made by defining four boundaries called walls in
PFC2D. In the first stage of creating the sample, these walls are fixed. After the walls have been defined, the particles are generated.

Figure 2.4: Random particle generation of particles with reduced radius.

To generate the particles, the user has to give a minimum and a maximum radius $r_{min}$ and $r_{max}$ and an initial porosity $n$. This (two-dimensional) porosity is chosen in such a way that the sample is nicely compacted after generation and the stress on the wall is not too large. A porosity of 0.12 has been used for this purpose. This value for porosity seems quite low. This is due to the 2D nature of the code (see Appendix VIII for a discussion on the issue of porosity and the differences between 2D and 3D porosity). The PFC2D program generates particles in a random way with a either linear or a Gaussian radius distribution. Here, a linear distribution is chosen. Then, the average particle radius can be calculated, which is $r_{av} = (r_{min} + r_{max})/2$. From this, the average area of each particle is $A_{av} = \pi (r_{av})^2$.

When the space enclosed by the four walls has an area of $A_{cel}$, the total number of particles $N$ can be calculated from the porosity, namely $N = (n-1)A_{cel}/A_{av}$. The quantity on the right hand side is truncated to obtain an integer value for $N$. Now, it is difficult to randomly put the particles in the area enclosed by the four walls, therefore the particles are first generated with a radius which is a factor 1.6 smaller than given. But, of course, the particles still have the same relative radius distribution. With their reduced radius, the PFC2D program can randomly generate the $N$ particles inside the area enclosed by the four walls, see Figure 2.4.

The particles are generated together with their stiffness characteristics, which must be given by the user in the form of either a normal and shear stiffness $k^n$ and $k^s$ in case of the linear contact model, or the microscopic shear modulus $G_m$ and poisson's ratio $\nu_m$ needed for the non-linear Hertz-Mindlin model. After the particles have been generated, the radii are expanded by the factor 1.6 to have their
intended size. During this process, the friction coefficient $\mu$ is set to zero, so there is no shear force present and particles can slide against each other to obtain a well compacted and more homogeneous sample, see Figure 2.5.

![Figure 2.5: Sample after radius multiplication to original particle size.](image)

Now, the sample is brought to an initial stress state defined by the user. The vertical stress on the bottom and top walls, and the horizontal stress on the left and right walls can be set to different values. In this process the friction coefficient $\mu$ is set to the original value specified by the user, and the material has the characteristics as intended. The way the PFC2D program creates the stress state is by freeing the walls and giving them a velocity normal to the walls according to the difference of the desired stress at that wall from the actual stress. At each time step a new velocity is calculated and eventually an equilibrium condition is reached where the stress is within a certain range close to the desired stress, see Figure 2.6. This way of sample generation and application of initial stress was also used for the biaxial test simulations, see appendix VII.
Figure 2.6: Initial stress state with externally applied stresses $\sigma_{xx}$ and $\sigma_{yy}$. Black lines are the normal contact forces between the particles.

The externally applied stress remains constant during the whole fracturing simulation, and the walls move accordingly to realise this boundary condition when for example fluid is injected into the borehole and it expands.
3 Used parameters for particles and fluid flow

3.1 Particle and wall parameters

Hydraulic fracturing experiments at GeoDelft and TU Delft were performed with the Swedish Baskarp sand. In the earlier performed biaxial test simulations, parameters have been found that model the behaviour of this Baskarp sand quite well, see Appendix VII. Parameters that resulted in a material that resembles Baskarp sand were found for both the non-linear Hertz contact model and the linear contact model. In biaxial test simulations for a wide range of confining stresses, the Hertz-model was found to have a more realistic behaviour. Therefore, the Hertz model has been used in the current hydraulic fracturing simulations.

The Hertz model parameters that resulted in a material resembling the Swedish Baskarp sand are presented in Table 3.1.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>shear modulus $G_m$ [GPa]</td>
<td>39</td>
</tr>
<tr>
<td>poisson’s ratio $\nu_m$</td>
<td>0.16</td>
</tr>
<tr>
<td>friction coefficient during biaxial test $\text{fric}$</td>
<td>1.3</td>
</tr>
<tr>
<td>friction during assembly and applying initial stress state</td>
<td>0.05</td>
</tr>
<tr>
<td>porosity $n$</td>
<td>0.12</td>
</tr>
<tr>
<td>maximum radius/minimum radius</td>
<td>4/3</td>
</tr>
</tbody>
</table>

Table 3.1: Hertz model parameters and additional parameters for generation of a sample best resembling Swedish Baskarp sand.

Note that the original parameters in the biaxial test simulations were found for a maximum radius/minimum radius ratio of 4:1, see Appendix VII. But it also was found that for smaller ratio’s the characteristics of the sample didn’t change as long as the ratio didn’t come very close to 1:1 where all particles have the same radius. A ratio of 4:3 still gave very good results. For the hydraulic fracturing simulations including fluid flow it’s better not to have great differences in particle radius in the model to obtain a more stable flow behaviour. A large variety in particle radius can cause some flow domains to be much smaller in volume than the domains in the rest of the sample. Then the fluid flow time step size has to be smaller to enable stable flow behaviour for these domains and these small domains entirely determine the maximum allowable flow time step size.

Besides particle parameters there are also parameters for the walls (boundaries of the sample). During the sample creation and fracturing simulation, the shear and normal stiffness of the walls were both taken $1.0 \times 10^9$ Pa and the wall friction was set to zero to have minimum influence of the boundary on the stress situation.

3.2 Fluid flow parameters

Besides the parameters for particles and walls, the fluid must also be characterised to be able to run the hydraulic fracturing simulations. As has been described in the report on fluid flow (Appendix VIII), there are three general parameters that describe the fluid flow. These are the fluid
bulk modulus $K$, the ratio of the intrinsic permeability to the viscosity $\kappa/\mu$, and the porosity $n$. The used parameters are presented in Table 3.2.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>fluid bulk modulus $K$ [GPa]</td>
<td>2</td>
</tr>
<tr>
<td>Permeability/viscosity ratio: $\kappa/\mu$ [m$^2$/sPa]</td>
<td>1.0E-8</td>
</tr>
<tr>
<td>Porosity $n$</td>
<td>0.4</td>
</tr>
<tr>
<td>flow time step dt_flow [s]</td>
<td>1.0E-5</td>
</tr>
</tbody>
</table>

Table 3.2: used parameters for fluid flow.

The fluid bulk modulus is that of pure water and the porosity of 0.4 is a realistic value for loose sand. For the ratio of intrinsic permeability to the viscosity, a value realistic for water flowing through sand has been used, namely a dynamic viscosity of 10E-3 Pas and an intrinsic permeability of 10 Darcy (10E-11 m$^2$). This doesn’t limit the fracturing simulations. A change in viscosity has merely an effect on the time-scale of the simulation, because a combination of borehole injection rate and the $\kappa/\mu$ ratio determines the overall flow behaviour.

The end time of the performed hydraulic fracturing simulations in this report was about 3E-3 s, which is very short. But for a viscous oil or gel the viscosity can be in the order of 100 Pas, a factor of 1.0E5 higher than the used value. Then, a simulation with the injection rate a factor 1.0E5 lower and the flow time step a factor 1.0E5 higher, would give exactly the same simulation results, the only difference being the time-scale. The end time would now be 300 seconds, a realistic value for the fluid used.

Note that, in Table 3.2, the chosen flow time step dt_flow is very small. Since fluid flow is implemented with a numerically explicit integration scheme, the time step needs to be very small for stability. The stable time step is found to be proportional to the average pore volume of the domains divided by the bulk modulus and permeability/viscosity factor, in other words proportional to $n\mu/(\kappa K)$. This means that for a factor 1.0E5 higher viscosity, indeed a factor 1.0E5 larger flow time step can be used and the viscosity determines essentially the time-scale of the simulation when the injection rate is scaled at the same time.

Further, it has been mentioned before (Table 3.1) that the porosity of the particle assembly was 0.12. This is the two-dimensional porosity used for the particle generation. This porosity is very low compared with a realistic porosity for an actual sample. The issue of porosity and the differences between 2D and 3D porosity has been extensively discussed in Appendix VIII. To have a more realistic fluid flow behaviour in sand, the fluid flow calculation is done with a porosity of 0.4.
4 Set-up of the hydraulic fracturing simulations

4.1 Model generation and fracturing simulation

A sample is generated according to the procedure described in section 1.3 using the particle parameters presented in the previous Chapter. The area modelled is a square of 20x20 meters. Most simulations were performed with 3450 particles before removal of the borehole. It has to be mentioned that not the actual sand grains are simulated with this model. Distinct particles are used in the hope to obtain a macroscopic behaviour that represents the macroscopic behaviour of sand while using much less microscopic particles than are present in an actual sand sample. In the next Chapter, the influence of particle size will be investigated to see to what extend this assumption is valid. After the model with certain initial stress state (Figure 2.6) has been created, a borehole with a radius of 0.5 m is created by removing particles within a circular region in the centre of the model. In the simulations performed with 3450 particles before removal of the borehole, approximately 30 particles in the centre circle were removed to create the borehole (Due to the randomness of the particle generation this removed number varies slightly). This removal is done without deformation calculation, otherwise the borehole would collapse under the influence of the applied external stress.

Before making equilibrium with a deformation calculation, the domain structure is created. Figure 4.1 shows this domain structure in a region around the borehole.

![Figure 4.1: Domain structure for fluid flow around the borehole. Domains are irregular in shape and the borehole is one domain.](image_url)

After the domains are created, a pressure of zero is applied to all domains except the borehole to which a pressure \( P_0 \) is applied. \( P_0 \) has a value larger than the average applied external stress to prevent collapse of the borehole. In the current hydraulic fracturing simulations, the value \( P_0 = \frac{3}{4}(\sigma_{xx} + \sigma_{yy}) \) has been taken, which is 1.5 times the average external stress. After this pressure is applied, the deformation calculation is made until equilibrium is reached with the external applied stress. The
fluid pressure in all the domains (including the borehole) is kept constant while deformation takes place. The equilibrium state is presented in Figure 4.2 and is the start of the hydraulic fracturing simulations.

![Figure 4.2: Initial state for the fracturing simulations with borehole (fluid) pressure $P_0$ 1.5 times the average applied external stress. The fluid pressure outside the borehole is zero.](image)

Now the hydraulic fracturing simulation can be run. For the fluid flow part, the flow time step, fluid bulk modulus, $\kappa/\mu$ ratio, and porosity presented in Table 3.2 of the previous section have been used. Also, since the current hydraulic fracturing simulations are controlled by the injection rate, the fluid injection rate must be given (in $[\text{m}^3/\text{ms}]$ because of the 2-dimensionality of the simulation). In most simulations we use an injection rate of 1000 $\text{m}^3/\text{ms}$. Then as boundary conditions for fluid flow we keep the pressure in the domains within 1 m distance from the boundaries (walls) fixed at a pressure of zero. Doing this simulates a drained hydraulic fracturing test.

The user also has to specify the number of flow steps to determine the total calculation time. The time scale of the simulation is determined by the flow steps. One flow step is done according to the presented fluid flow method. During this flow step, also a certain volume of borehole fluid is injected. After the flow step, the fluid pressures have changed. Now an equilibrium needs to be made by doing a number of deformation steps. The condition for equilibrium is that the ratio of the average unbalanced force of all particles divided by the average contact force of all contacts has to be lower than a value given by the user. The number of steps needed to obtain equilibrium depends on several factors and is different for each flow step. When a fracture is generated more steps are needed for equilibrium. As mentioned earlier, during the deformation there is only coupling of the borehole. In other words, the pressure in the domains doesn’t change during deformation (unless breaking of
contacts happens and new domains are created from merging or splitting of old ones) except for the borehole for which fluid pressure drops with expansion during deformation stepping.

When a fracture propagates from the borehole, contacts are breaking and the borehole domain expands. Example results of fracture patterns, pressure distributions and normal contact force distributions during a hydraulic fracturing simulation are given in Appendix I. Nicely visible is the infiltration of fluid pressure during the simulation. At the same time, the normal contact force in this pressure-infiltrated zone around the borehole decreases as a result.
5  Accuracy, particle size dependence and computation times of the fracturing calculations

In this chapter, two aspects of the hydraulic fracturing simulations are studied: the accuracy and the influence of particle size. Further, the computation times are monitored to find out the limits of the current code.

To study the above mentioned aspects, two sets of hydraulic fracturing simulations were performed, each with the parameters and model geometry as discussed in the previous Chapters. One set of simulations has been done with 3450 particles and the other set of simulations was made with a reduced (average) particle radius of half the radius used in the first set of simulations resulting in 13802 particles, which is about four times as much particles. In the report on the PFC2D biaxial test simulations (see Appendix VII), it has been shown that the stiffness characteristics of a sample with more particles don’t change significantly. Therefore, these simulations can be used to observe the dependence of fracturing behaviour on particle size. All the simulations were made with a vertical applied stress of 1.2 bar and a horizontal applied stress of 0.8 bar. The borehole injection rate was 1000 m³/ms.

For each of the two models several simulations were performed for different equilibrium criteria. As mentioned in the previous chapter, the condition for equilibrium is that the ratio of the average unbalanced force of all particles divided by the average contact force of all contacts has to be lower than a value given by the user. For the model with 3450 particles, ratio’s of 1%, 0.5%, 0.25% and 0.125% were used. For the model with 13802 particles, ratio’s of 1%, 0.5% and 0.25% were used.

The results of the calculations are presented in Appendix II. First the borehole pressure versus time, borehole deleted contacts versus time graphs are shown for the various simulations and then the fracture patterns at the end of the simulations done with 1% relative unbalance ratio are presented.

In the first graph of Appendix II, the borehole pressure versus time graph for the simulations with 3450 particles, it can be seen that the simulations differ considerably in peak pressures. Lower accuracy (1% relative unbalance) results in higher peak pressure. The simulations with 0.25% and 0.125% don’t differ significantly in peak pressure anymore, hence it’s assumed that a convergence has been reached. Less flow steps were used for simulations with higher accuracy because they need more iterations. The calculations ran until the peak pressure had been reached to compare accuracy.

The second graph in Appendix II shows the borehole pressures for the simulations with 3450 and 13802 particles simultaneously. Here it can be seen that the simulation with more particles and a relative unbalance of 1% gives a much higher peak than the simulation with less particles for the same unbalance of 1%. This is understandable because the highest unbalanced forces in these hydraulic fracturing simulations appear in the vicinity of the borehole. Therefore, in the model with more particles, there are relatively more particles far away from the borehole and these particles have almost no unbalanced forces so that the average unbalanced force of all particles is comparatively low in case of more particles. In the graph it’s visible that for the 13802-particles model the simulation with 0.5% relative unbalance is close to the 1% situation for simulation with 3450 particles.

An overview of peak borehole pressures for the various simulations is presented in Table 5.1:
Table 5.1: Comparison of peak borehole pressures for the two sets of simulations.

<table>
<thead>
<tr>
<th>Relative unbalanced ratio</th>
<th>Peak borehole pressure [bar] for 3450 particle simulation</th>
<th>Peak borehole pressure [bar] for 13802 particle simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1%</td>
<td>3.57</td>
<td>4.85</td>
</tr>
<tr>
<td>0.5%</td>
<td>3.21</td>
<td>3.65</td>
</tr>
<tr>
<td>0.25%</td>
<td>2.92</td>
<td>3.32</td>
</tr>
<tr>
<td>0.125%</td>
<td>2.89</td>
<td>-</td>
</tr>
</tbody>
</table>

The third graph in Appendix II shows borehole pressure and deleted borehole contacts versus time plot for the 0.25% unbalance, 13802 particles simulation and the 0.5% unbalance, 3450 particles simulation. The simulations have similar peak pressures as mentioned before, and it’s also visible that the slope of borehole pressure versus flow time curves are very similar. This indicates that the stiffness characteristics of the two samples are nearly identical as was also found in the biaxial test simulations (Appendix VII).

Also in the third graph it can be seen that the fracturing behaviour of the two samples is different. At a flow time of $1.5 \times 10^{-4}$ s, a number of contacts in the borehole breaks for the simulation with more particles. This is also about the same time the peak pressure has been reached. The fracture is thus initiated at about the same time the peak pressure is reached. But for the model with 3450 particles, the first contact in the borehole breaks at $4.7 \times 10^{-4}$ s, a while after the peak pressure has been reached. In the fourth graph of Appendix II, the deleted contacts for the 1% relative unbalance simulations are also shown, which were made for a longer flow time interval (due to the need of less iterations). For the 3450 particle model, several borehole contacts break at $1.2 \times 10^{-3}$ s, indicating a fracture which is indeed long after the peak pressure has been reached. Another thing visible in this graph is that the breaking of contacts for the simulations with higher accuracy is not noticeably different from the simulations of lower accuracy indicating a similar fracturing behaviour.

Also in Appendix II the fracture patterns at the end of the two simulations with 1% relative unbalance are shown. The fracture for the original particle size simulation is short and wide, while the fracture of the reduced particle size simulation is long and narrow, it propagates faster. The reduced particle size simulation was run up to a flow time of $1.5 \times 10^{-3}$ s, while the simulation with 3450 particles was run up to a flow time of $3.0 \times 10^{-3}$ s. Therefore, in the latter the total injected volume in the borehole is twice that of the reduced particle size simulation. This means that the total fracture volume in the reduced particle size simulation has to be lower even though the fractures are longer. This must be due to the narrower fracture width. Another thing is that in the borehole pressure versus flow time graphs it can be seen that, after the peak, the pressure drops faster for the reduced particle size simulation. This could be related to the faster fracture propagation. In the reduced particle size simulations the fractures have propagated so far into the sample that in this case probably the edges (where the external applied stress is acting) influence the simulation.

The question is still why the fractures of the reduced particle size simulation are narrower. From the simulations it appears as if the fracture width is similar to the particle diameter. To investigate this effect, it would be interesting to see the results for another size reduction, but the current calculation time is about 11 days for the reduced particle size simulation. This is already a factor of 10 longer
than the simulation with the coarser sample having four times less particles. This leaves further size reduction with the current hydraulic fracturing implementation in PFC2D out of reach.

5.1 Computation times

The calculations were performed with a Pentium III 550 MHz. The table below shows calculation times for the various simulations:

<table>
<thead>
<tr>
<th>simulation</th>
<th>number of flow steps</th>
<th>computation time</th>
<th>average time per flow step</th>
</tr>
</thead>
<tbody>
<tr>
<td>1% unbalance, 3450 particles</td>
<td>300</td>
<td>1 day 18 hours</td>
<td>8.4 minutes</td>
</tr>
<tr>
<td>1% unbalance, 13802 particles</td>
<td>150</td>
<td>11 days 16 hours</td>
<td>1.9 hours</td>
</tr>
<tr>
<td>0.25% unbalance, 3450 particles</td>
<td>47</td>
<td>22 hours</td>
<td>28 minutes</td>
</tr>
<tr>
<td>0.25% unbalance, 13802 particles</td>
<td>33</td>
<td>4 days and 8 hours</td>
<td>3.2 hours</td>
</tr>
<tr>
<td>0.125% unbalance, 3450 particles</td>
<td>33</td>
<td>23 hours</td>
<td>42 minutes</td>
</tr>
</tbody>
</table>

The simulation with 13802 particles is too large to do parameter studies, since it takes a long time to run, especially for a satisfactory unbalance (0.125% or 0.25%). The simulations for the coarser sample will therefore be used to do the parameter studies in this report. These will be made with a relative unbalanced ratio of 0.25%, since this has shown to be sufficiently accurate.

The main time consuming aspect of the simulations is that after each flow step a number of deformation steps is necessary to make equilibrium and after each deformation step the pressure in the borehole domain and fluid force on all the particles has to be re-evaluated. This is all done in PFC’s FISH interpreter language. Although the fluid pressure in all domains except the borehole remains the same, the deformation might change the shape of a domain and direction of the force, especially when fractures appear, so the fluid force must be calculated for all the particles.
6 Hydraulic fracturing results for different random samples

In the previous chapter, simulation accuracy has been established and it was observed that peak pressures didn’t differ too much between samples of different particle sizes. Here, for four different random samples with 3450 particles simulations will be compared at 10 bar confining stress to see what differences can occur in samples essentially generated in the same way with only different particle distributions.

The simulations were performed with an relative unbalanced force criterion of 0.25%, using the particle and fluid flow parameters as discussed in Chapters 3 and 4. Starting with different seeds for the random generator, four different samples were generated while using the same particle size distribution for the particles. There are basically two random processes. One to select a particle radius from the size distribution and one to position the particle in the designated area.

The results of the simulations are presented in Appendix III First the borehole pressure versus time curves are shown and then the fracture patterns at the end of the simulations are displayed.

From the borehole pressures versus time plot, the peak pressures as well as the number of broken contacts in the borehole at the end of each calculation can be determined. The results are given in Table 6.1:

<table>
<thead>
<tr>
<th>Starting seed random generator</th>
<th>peak borehole pressure [bar]</th>
<th>maximum number of deleted contacts in borehole</th>
<th>Factor of peak pressure/ conf. stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>10001</td>
<td>37.7</td>
<td>8</td>
<td>3.77</td>
</tr>
<tr>
<td>16101</td>
<td>37.0</td>
<td>12</td>
<td>3.70</td>
</tr>
<tr>
<td>5023</td>
<td>35.8</td>
<td>8</td>
<td>3.58</td>
</tr>
<tr>
<td>10000</td>
<td>39.5</td>
<td>10</td>
<td>3.95</td>
</tr>
</tbody>
</table>

Table 6.1: Results of hydraulic fracturing simulations at 10 bar confining stress using four samples generated starting from different seeds for the random generator.

It can be observed that there is about 10% difference in peak borehole pressure for the simulations. The fracturing patterns show noticeable differences. Sometimes one fracture and sometimes two fractures or three short fractures. Nevertheless, the behaviour of the borehole pressure and deleted contacts versus time curves shows the same trend in all cases with peak pressure reached at nearly the same moment and the same post-peak behaviour. Also the trend in broken contacts is very similar.
7 Influence of confining stress on hydraulic fracturing

To investigate fracturing behaviour for different confining stresses, the confining stress has been varied in four simulations. In the report on biaxial test simulations, included in Appendix VII, the behaviour of dry sand was tested under various confining stresses. It was observed that the non-linear Hertz contact model, with parameters as in Table 3.1, gave a realistic increase in Young’s modulus with increasing confining stress. The hydraulic fracturing simulations presented here were therefore made with the non-linear Hertz model. Further, the fluid flow parameters given in chapter 3 were used.

Four simulations have been made for confining stresses (horizontal and vertical stress equal) of 1 bar, 10 bar, 100 bar and 500 bar respectively. In all the simulations, the same injection rate of 1000 m$^3$/ms has been used and 300 flow steps were performed, thereby injecting the same volume of fluid. Because of the high bulk stiffness of the borehole fluid, the pressure in the borehole can be made significantly higher without much volume loss due to compression of the fluid. It is expected that the total volume of the borehole including fractures is approximately equal in the four simulations and good comparison of results is possible.

Results of the four hydraulic fracturing simulations are shown in Appendix IV. First the borehole pressure versus time plots are shown for each case, then the fracture patterns at the end of the calculation are displayed.

From the borehole pressure versus time plots, the peak pressures as well as the number of broken contacts in the borehole at the end of each calculation can be determined. The results are given in Table 7.1.

<table>
<thead>
<tr>
<th>vertical confining stress [bar]</th>
<th>peak borehole pressure [bar]</th>
<th>maximum number of deleted contacts in borehole</th>
<th>Factor of peak pressure/ conf. stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.79</td>
<td>9</td>
<td>3.79</td>
</tr>
<tr>
<td>10</td>
<td>39.5</td>
<td>10</td>
<td>3.95</td>
</tr>
<tr>
<td>100</td>
<td>345</td>
<td>14</td>
<td>3.45</td>
</tr>
<tr>
<td>500</td>
<td>1210</td>
<td>13</td>
<td>2.42</td>
</tr>
</tbody>
</table>

Table 7.1: Results for the hydraulic fracturing simulations at different confining stress.

From this table it can be seen that the factor of peak pressure divided by confining stress is fairly constant and becomes a little smaller at high stresses. This is to be expected since it was found that at higher stress, the sample is relatively softer. Then, with the same stress ratio of borehole pressure to confining stress, the expansion of the borehole is larger at higher confining stress due to the softer sample. This indicates earlier fracturing. Using cavity expansion theory, assuming as fracture criterion a certain amount of plasticity, it has also been found that at higher stress the ratio of limit pressure to confining stress reduces.

Another thing that’s apparent in the pressure versus time plots in Appendix IV, is that the peak pressure shifts to a later time for higher confining stresses. This is also due to the sample being relatively softer at higher confining stresses. The factor of peak pressure divided by confining stress is
almost constant. Then, the absolute increase in borehole pressure at high confining stress is far more than at low confining stress. Due to the relatively soft sample at higher stress, more expansion is needed to generate the required stresses in the soil. This requires more injection fluid to reach the peak borehole pressure.

Another interesting thing is that for the simulations at lower confining stresses, 1 bar and 10 bar, the fractures appear after the peak pressure has been reached, while for the simulations at higher confining stress fractures already appear before the peak pressure has been reached. An explanation for this could also be the relatively softer sample at higher stress. It has been shown that at lower confining stresses the borehole expansion is less at the moment of peak pressure than the expansion at peak pressure for higher confining stresses. More expansion could induce fractures even at lower ratio’s of borehole pressure to confining stress.


8 Influence of friction angle on fracturing behaviour

In this Chapter, a series of hydraulic fracturing simulations is described in which the friction coefficient $\mu$ has been varied. This friction coefficient determines the maximum possible shear force in a contact, which can be the $\mu$ times the magnitude of the normal contact force. If the shear force is about to exceed this value, sliding between particles occurs so the shear force will not increase. For a higher coefficient, the sliding occurs later and the material acts as one with a higher internal friction angle.

The simulations were made with the Hertz model and fluid flow parameters as presented in Chapter 3 and with the model geometry discussed in Chapter 4. The confining stress was taken 10 bar for both the horizontal and vertical directions to prevent collapse of the sample at low friction. The friction coefficient $\mu$ has been varied from 0.4 to 1.3. From this friction coefficient, an internal friction angle for the particles itself can be determined from $\phi = \arctan(\mu)$. This is a microscopic friction angle. It has been observed in the biaxial test simulations (Appendix VII), that the macroscopic friction angle is lower. Thus, a set of biaxial test simulations has been performed at a confining stress of 10 bar, to obtain these macroscopic friction angles belonging to the various values of $\mu$. These friction angles were calculated using the method described in Appendix VII. The results of these biaxial test simulations are presented in Table 8.1.

<table>
<thead>
<tr>
<th>friction coefficient $\mu$</th>
<th>Particle friction angle $\arctan(\mu)$ calculated from [degrees]</th>
<th>Material friction angle from biaxial tests $\phi$ [degrees]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.3</td>
<td>52.4</td>
<td>34.5</td>
</tr>
<tr>
<td>0.9</td>
<td>42.0</td>
<td>31.1</td>
</tr>
<tr>
<td>0.7</td>
<td>35.0</td>
<td>30.6</td>
</tr>
<tr>
<td>0.4</td>
<td>21.8</td>
<td>26.1</td>
</tr>
</tbody>
</table>

Table 8.1: Used PFC2D friction coefficients and their corresponding internal friction angles for the particles and material friction angles (macroscopically) resulting from biaxial test simulations at 10 bar for different. Note that the macroscopic friction angles are lower.

Then, the fracturing simulations were performed. To investigate the influence of the friction coefficient only, the model generation was done only once and that model was used in all fracturing simulations. At the start of each simulation the friction was set to the desired value. Results of the four hydraulic fracturing simulations are shown in Appendix V. First the borehole pressure versus time plots are shown for each case, then the fracture patterns at the end of the calculation are displayed. The peak pressures and maximum number of broken contacts are given in Table 8.2.

<table>
<thead>
<tr>
<th>friction coefficient $\mu$</th>
<th>peak borehole pressure [MPa]</th>
<th>maximum number of deleted contacts in borehole</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.3</td>
<td>3.85</td>
<td>11</td>
</tr>
<tr>
<td>0.9</td>
<td>3.55</td>
<td>10</td>
</tr>
<tr>
<td>0.7</td>
<td>3.31</td>
<td>9</td>
</tr>
<tr>
<td>0.4</td>
<td>2.95</td>
<td>6</td>
</tr>
</tbody>
</table>

Table 8.2: Results of fracturing simulations for various friction coefficients.
For lower friction coefficients (smaller friction angles) the peak pressure drops slightly. From the graphs of borehole pressure versus time in Appendix V, it can be seen that the pressure curve also becomes more flat at lower friction angles. Namely there is not a definite peak visible but a range in which the pressure remains fairly constant. Also for lower friction angles less contacts break in the borehole. This is also visible in the fracture patterns in Appendix V. It can be seen that at high friction there is a nice distinct fracture, whereas at lower friction there is merely borehole expansion and not any significant fracturing. An explanation is that for lower friction the particles tend to redistribute themselves. Therefore, when a fracture would start to occur, the particles slide and redistribute easily at low friction angles thereby erasing the starting fracture. The effect is that the borehole expands fairly evenly without significant fractures at lower friction. At zero friction, no fractures can appear anymore.


9 Hydraulic fracturing for different injection rates

To determine the effect of infiltration, the fracturing behaviour is investigated for various borehole injection rates. If the injection rate is very low, the fluid pressure in the borehole won’t be able to build up high enough for a fracture to appear because of fluid flow through the borehole wall. If the injection rate is still low, but high enough to generate a fracture, the fluid pressure will have infiltrated far into the zone surrounding the borehole. For higher injection rates, the infiltration becomes less and less, because build-up of the pressure in the borehole is happening faster than pressure build-up through fluid flow (of course in a real experiment there may exist significant coupling of deformations with pore fluid which causes pressure build-up by borehole expansion, but this effect can currently not be described satisfactory with the simulations, see Appendix VIII). If the injection rate is very high, the soil surrounding the borehole acts like it’s impermeable and pressure infiltration due to fluid flow would be non-existing.

Although the model is incapable of describing fully coupled behaviour, the main objective of these variations of injection rate here is to investigate the peak borehole pressure for situations from no pressure infiltration to a large infiltrated zone.

The simulations were performed with the Hertz model and fluid flow parameters as given in Chapter 3 and the model geometry discussed in Chapter 4. The confining stress was 100 bar both horizontally and vertically. One model was generated and used in three calculations. One with injection rate 1000 [m³/ms], the next with injection rate 100 [m³/ms] and the last with injection rate 1000 [m³/ms], but where the permeability is zero. This last calculation is equivalent to having a very high injection rate in the current code.

The calculation with injection rate of 1000 [m³/ms] was performed with 300 flow steps. Then, the simulation with injection rate of 100 [m³/ms] needs to have 3000 flow steps of the same magnitude to have the same volume injected into the borehole. It turned out that the calculation was only stable if after each flow step a number of deformation steps were made. It was not possible to do 10 flow steps for example and then start finding an equilibrium. The result is that the calculation with 100 [m³/ms] injection rate took approximately 10 times as long (almost 4 days). This prevented from reducing the injection rate significantly again.

The simulation with zero permeability was performed with 300 steps because the injection rate was also 1000 [m³/ms] and it was known that this injection rate and borehole coupling could be correctly described in this way.

Results of the simulations are presented in Appendix VI. The peak pressures for the three cases are given in Table 9.1:

<table>
<thead>
<tr>
<th>case</th>
<th>peak pressure [bar]</th>
<th>peak press/conf. stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>impermeable</td>
<td>383</td>
<td>3.83</td>
</tr>
<tr>
<td>injection rate 1000 m³/ms</td>
<td>345</td>
<td>3.45</td>
</tr>
<tr>
<td>injection rate 100 m³/ms</td>
<td>303</td>
<td>3.03</td>
</tr>
</tbody>
</table>
Table 9.1: Peak pressures for hydraulic fracturing calculations with various injection rates.

From the fracture patterns in Appendix VI, it can be seen that for impermeable case the pressure outside the borehole remains zero, while for the lowest injection rate the sample is infiltrated (by pressure) to a large extent. In every case fractures appear although the fracturing seems less clear for the low injection rate case. The peak pressure drops somewhat for lower injection rates.
10 Comparison of simulation results with experiments

In the previous chapters, hydraulic fracturing simulations have been performed for a variety of cases. This Chapter presents some results from the literature and results of hydraulic fracturing experiments performed at TU Delft and GeoDelft, to compare them with the simulation results.

10.1 Hydraulic fracturing experiments at GeoDelft and TU Delft

The TU Delft experiments were performed at confining stresses ranging from 70-200 bar. A brief overview of the experiments was presented in [DelFrac 2001]. The experiments where fractures appeared and where no strange anomaly have been observed are listed in Table 10.1:

<table>
<thead>
<tr>
<th>Test</th>
<th>Fluid</th>
<th>Radial stress [MPa]</th>
<th>Axial stress [MPa]</th>
<th>Stress ratio P max/radial</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>BHS05</td>
<td>Viscasil 500</td>
<td>7.5</td>
<td>12.5</td>
<td>3.6</td>
<td>fractures started from ends</td>
</tr>
<tr>
<td>BHS06</td>
<td>Viscasil 500</td>
<td>7</td>
<td>10</td>
<td>3.2</td>
<td>fractures started from ends</td>
</tr>
<tr>
<td>BHS10</td>
<td>Borate X-linked HPG-gel 50 lb/1000 gal</td>
<td>1.6</td>
<td>2.7</td>
<td>4.3</td>
<td>small fractures at various levels</td>
</tr>
<tr>
<td>BHS11</td>
<td>Viscasil 500</td>
<td>5</td>
<td>7</td>
<td>4.2</td>
<td>two fractures (oblique to vertical) starting from bottom of injection section</td>
</tr>
<tr>
<td>BHS12</td>
<td>Borate X-linked HPG-gel 50 lb/1000 gal + quartz powder</td>
<td>7</td>
<td>12</td>
<td>3.4</td>
<td>fractures started from bottom</td>
</tr>
<tr>
<td>BHS13</td>
<td>Borate X-linked HPG-gel 50 lb/1000 gal + quartz powder</td>
<td>19.5</td>
<td>28</td>
<td>2.9</td>
<td>fractures started from bottom</td>
</tr>
</tbody>
</table>

Table 10.1: Results of fracture tests on sand at high confining stress performed at TU Delft [DelFrac 2001].

The radial stress in Table 10.1 can be seen as the confining stress in the fracturing simulations, and the ratio of peak pressure to radial stress can be compared to the peak pressure divided by confining stress ratio’s found in the Chapter 7.

Experiments at GeoDelft, [GD 1999], showed factors of peak pressure divided by vertical (maximum) confining stress from 1.9 to 2.3. These tests were performed at a vertical confining stress of 2 bar. The experiments were not performed under the same symmetry as the TU Delft experiments. The “borehole” was aligned horizontally and therefore the situation is more akin’ to the simulations performed in Chapter 5, with different horizontal and vertical applied stress. But if we assume that the horizontal stress in the experiments is 2/3 of the vertical stress and that the minimum confining stress (the horizontal) in this case determines the fracturing, we can compare results with the simulations in Chapter 7 together with the TU Delft experiments by dividing the peak pressures by the estimated...
horizontal stress. In doing so, we find ratio’s of peak pressure to horizontal stress, ranging from 2.8 to 3.4.

Figure 10.1 shows the results from the hydraulic fracturing tests performed at TU Delft and GeoDelft as well as the results for the simulations made in Chapter 7 for various confining pressures (isotropic):

![Figure 10.1: Simulation results of pressure ratio's for different confining stress compared with the TU Delft hydraulic fracturing results and the dry sample results from [Alsiny et al. 1992].](image)

The results of the TU Delft experiments are in good agreement with these simulations. Also visible from both Table 10.1 and Figure 10.1 is that the general trend of the TU Delft experiments is that at higher confining stress the ratio of peak pressure divided by confining stress becomes smaller. This is also in accordance with the simulations (at higher confining stresses) and the cavity expansion theory as mentioned previously. The GeoDelft experimental results are somewhat lower than the simulation results. This could be due to the uncertainties in horizontal confining stress. As mentioned, the GeoDelft experiments are more akin to the simulations performed in Chapter 5 where a vertical confining stress of 1.2 bar and a horizontal confining stress of 0.8 bar were used. In the simulations a peak pressure was found (unbalance criterion of 0.125%) of 2.89 bar, hence the peak pressure divided by vertical confining stress gives a factor of 2.4, in better agreement with the factors 1.9 to 2.3 found in the GeoDelft experiments. Also there was a large infiltration zone present in the GeoDelft experiments which is perhaps more like the simulations at lower injection rates as shown in the previous Chapter. For these simulations, the peak pressure was also slightly lower.

Also plotted in Figure 10.1 are results from [Alsiny et al. 1992] who performed cavity expansion experiments on a dry sample. These results show clearly higher peak pressures than the hydraulic fracturing experiments and simulations. Maybe this is due to the presence of a membrane in the borehole, making distinct fractures impossible. The dry sample results show a few further interesting features which will be described below.
10.2 Tests on dry sand sample

The mentioned experiments of [Alsiny et al. 1992] are cavity expansion tests on a dry cylindrical sand sample under plane strain conditions. There was a membrane present in the hole of the sample and fluid was injected into the hole, leading to cavity expansion with no fluid infiltration. The experiments were conducted with external (radial) applied pressures of 0.5-2.0 bar. Figure 10.2 shows some results of [Alsiny et al. 1992].

![Figure 10.2: Experimental results from [Alsiny et al. 1992].](image)

The figure shows $\sigma_c/\sigma_0$ as a function of increase of cavity volume during the test, where $\sigma_0$ is the confining stress and $\sigma_c$ is the differential cavity pressure which is the actual cavity pressure $P$ minus the confining stress, therefore $P/\sigma_0 = \sigma_c/\sigma_0 + 1$. This was used to convert the results and present them in Figure 10.1. In Figure 10.2, the peak values of $\sigma_c/\sigma_0$ range from 4.2 to 4.5, so the maximum cavity pressure divided by confining stress ranges from 5.2 to 5.5.

As mentioned earlier, the Alsiny experiments contained a membrane, which has a certain stiffness and which is not present in the hydraulic fracturing experiments and simulations. Hence, the fluid doesn’t penetrate in a fracture. In their experiments, [Alsiny et al. 1992] observed shear bands around the borehole, see Figure 10.3. And there was an irregular cavity expansion, but no hydraulic fractures were created.

There seems to be a difference between pure cavity expansion and hydraulic fracturing, and cavity expansion shows higher peak pressures than hydraulic fracturing. Alsiny’s results were higher than the fracturing experiments and simulations, as was shown in Figure 10.1. However, care must be taken here, since it has to be mentioned that the characteristics of the sand from the Alsiny experiments could not be directly matched to the modelled sand of PFC2D, which might yield somewhat different results.
Aside from this, it’s interesting to observe from Figure 10.2 that for higher confining stress the peak shifts to the right, meaning that, at higher confining stress, there is more increase in cavity volume (before fracturing) for the same $\sigma_c/\sigma_0$ ratio. This corresponds with the simulation results from Chapter 7, given in Appendix IV, where the pressure peak occurred at a later flow time at higher confining stresses, and therefore at a time when more volume was injected into the borehole. The explanation is that this is because at high confining stress, the stiffness of the sample is relatively lower (relative to the magnitude of the increase in borehole pressure), and the pressure build-up is slower. Therefore, more expansion is needed to generate a certain borehole wall pressure.
11 Conclusions and recommendations

Hydraulic fracturing simulations have been performed with the distinct element code PFC2D. For this purpose, fluid flow has been added in the code with special routines, and also the updating of flow domains when fractures appear has been implemented in the code. Parameter studies have been done resulting in the following observations:

- The choice of particle size does not affect the peak pressures found in the simulations, if a small enough unbalance criterion is used. Smaller particles do, however, give a different fracturing behaviour. Simulations with smaller particles give longer and narrower fractures than simulations with larger particles. The fracture width seems to be in the order of the particle size. Due to the already large computation times it has not been possible to further reduce the particle size and see the results. It is also uncertain if the fracture width has anything to do with PFC2D’s handling of the breaking of contacts.
- At higher confining stresses, the ratio of peak borehole pressure to confining stress in the hydraulic fracturing simulations decreases with increasing confining stress. This trend was also observed in experiments.
- The peak borehole pressure occurs at a later time (a higher injected volume) for higher confining stress. This was also observed in experiments.
- In the simulations at lower confining stress, the peak borehole pressures occurred before the appearance of fractures, while at higher confining stress already many contacts break before the peak pressure has been reached.
- A lower internal friction angle leads to a less distinct fracture pattern in loose sand, because particles redistribute more easily, filling a fracture after it has been formed. Lower friction angles give also slightly lower peak borehole pressures.
- At higher injection rates or a more impermeable behaviour of the sample, the peak pressure is slightly higher than for lower injection rates where a large zone of pressure infiltration around the borehole is present.
- Quantitatively, the peak pressures found in the hydraulic fracturing simulations at different confining stresses, agree well with the hydraulic fracturing experiments done at TU Delft in 2001[DelFrac 2001]. The peak pressure to confining stress ratio’s in the GeoDelft experiments are somewhat lower than calculated. This could be due to uncertainty in the actual horizontal confining stress or perhaps because a large infiltrated zone was present in the GeoDelft experiments, which according to numerical results would also yield lower peak stress.
- Dry sample cavity expansion tests, [Alsiny et al. 1992], show significantly higher peak pressures than the hydraulic fracturing experiments and simulations. In Alsiny’s experiments, shear bands were found, other than hydraulic fractures. Pure cavity expansion and hydraulic fracturing seem different. Pressures obtained from cavity expansion theory also overestimate the peak pressures found in hydraulic fracturing.

The hydraulic fracturing simulations are able to model the hydraulic fracturing process in a satisfactory way and showed good agreement with experimental results, both trend-wise and quantitatively. It is recommended to investigate further the particle size effects of the simulations to know the value of the simulations with larger particles, which are more practical computationally. To
do these kind of simulations, the issue of large computing time has to be overcome, which is a complicated task in the PFC2D program as it is now.

Also, the current implementation of hydraulic fracturing could be extended to model fracturing for samples with cohesion. Such investigations can further increase the application range of the current code for hydraulic fracturing simulations.
12 References

[Alsiny et.al. 1992]

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Period 1st of May 2001 to 1st of November 2001
Date 24 November 2001, section “Fracturing test on sand at high stress”

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‘Blow out proeven’
GeoDelft report, CO381070/9, September 1999

[Itasca 1999]
PFC2D manuals: ‘Theory and background”, “Fish reference guide”
Itasca 1999
APPENDICES
APPENDIX I

Example of the results from a hydraulic fracturing simulation. Fracture patterns and normal contact forces at different flow times.
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Confining stress 10 bar, different random samples

<table>
<thead>
<tr>
<th>flow_time during calculation [s]</th>
<th>number of deleted contacts in borehole</th>
<th>p [Mpa]</th>
</tr>
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<tbody>
<tr>
<td>0.0E+00</td>
<td>0.0E+00</td>
<td>0.0E+00</td>
</tr>
<tr>
<td>5.0E-04</td>
<td>5.0E-04</td>
<td>5.0E-04</td>
</tr>
<tr>
<td>1.0E-03</td>
<td>1.0E-03</td>
<td>1.0E-03</td>
</tr>
<tr>
<td>1.5E-03</td>
<td>1.5E-03</td>
<td>1.5E-03</td>
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<tr>
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</tr>
<tr>
<td>3.0E-03</td>
<td>3.0E-03</td>
<td>3.0E-03</td>
</tr>
</tbody>
</table>

- deleted contacts seed 10001
- deleted contacts seed 16101
- deleted contacts seed 5023
- deleted contacts seed 10000
- borehole pressure seed 10001
- borehole pressure seed 16101
- borehole pressure seed 5023
- borehole pressure seed 10000
Fracture patterns at the end of the simulations (with 0.25% relative unbalance) for the four different random samples. Shades represent fluid pressure. Dark blue is zero while the red is the maximum pressure (which is in the borehole)
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Confining stress 1 bar

Confining stress 10 bar
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Confining stress 100 bar

Confining stress 500 bar
Fracture patterns (zoomed in around bore hole) at the end of the simulation for different confining stresses. Shades represent fluid pressure. Dark blue is zero while the red is the maximum pressure (which is in the borehole)

\[ \sigma_{xx} = 1 \text{ bar}, \sigma_{yy} = 1 \text{ bar} \]

\[ \sigma_{xx} = 10 \text{ bar}, \sigma_{yy} = 10 \text{ bar} \]

\[ \sigma_{xx} = 100 \text{ bar}, \sigma_{yy} = 100 \text{ bar} \]

\[ \sigma_{xx} = 500 \text{ bar}, \sigma_{yy} = 500 \text{ bar} \]
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Appendix V: Results for different friction coefficients

**friction coefficient=1.3**

- Deleted contacts
- Borehole pressure
- Confinement stress

**friction coefficient=0.9**

- Deleted contacts
- Borehole pressure
- Confinement stress
Appendix V: Results for different friction coefficients

For friction coefficient = 0.7:

- Deleted contacts
- Borehole pressure
- Confinement stress

For friction coefficient = 0.4:

- Deleted contacts
- Borehole pressure
- Confinement stress
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Fracture patterns at the end of the simulation for different friction coefficients. Shades represent fluid pressure. Dark blue is zero while the red is the maximum pressure (which is in the borehole)

\( \mu = 1.3, \varphi = 34.5^\circ \)  \hspace{1cm}  \( \mu = 0.9, \varphi = 31.1^\circ \)

\( \mu = 0.7, \varphi = 30.6^\circ \)  \hspace{1cm}  \( \mu = 0.4, \varphi = 26.1^\circ \)
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impermeable case with injection rate 1000 m³/ms

injection rate 1000 m³/ms
Appendix VI: Results for different injection rates

Injection rate 100 m$^3$/ms, permeability 1.0 E-8 m$^2$/sPa

Flow time during calculation [s]

Deleted contacts
Borehole pressure
Confining stress
Appendix VI: Results for different injection rates

Fracture patterns at the end of the simulation for different injection rates. Shades represent fluid pressure. Dark blue is zero while the red is the maximum pressure (which is in the borehole).

impermeable case

injection rate = 1000 $m^3/\text{ms}$

injection rate = 100 $m^3/\text{ms}$
APPENDIX VII
GeoDelft report ‘Biaxial test simulations with PFC2D’
Biaxial test simulations with
PFC2D

CO386730/05  version 2
January 2002
Biaxial test simulations with PFC2D

CO386730/05
January 2002
N:\projecten.afd\386730 - Hydraulic

The survey was performed for:
DELFRAK CONSORTIUM
DELTFT

DEPARTMENT STRATEGIC RESEARCH
Project manager : ir. A. Bezuijen
Project supervisor : dr.ir. P. van den Berg

GeoDelft
Stieltjesweg 2, 2628 CK DELFT
Postbus 69, 2600 AB DELFT
The Netherlands

Telephone (+31) 15 - 269 35 00
Telefax (+31) 15 - 261 08 21
Postal account 234342
Bank MeesPierson NV
Account 25.92.35.911
In this report, biaxial tests are simulated with the two-dimensional discrete element code PFC2D from Itasca. The calculations were made for non-cohesive materials. Therefore, the behaviour of the particles does not include bonding. The main objective of the calculations is to determine which micro parameters should be chosen to achieve a certain macro-behaviour. To understand the influence of a specific micro parameter, first some simulations are made to see if the change in one of the micro parameters has a major effect on all of the macro parameters (stiffness, poisson’s ratio, angle of internal friction and angle of dilatancy) or of just one.

When the influence of each micro parameter is known, this knowledge is then applied to adjust the micro parameters in such a way that the macro parameters resulting from the biaxial test simulation are similar to those of Swedish ‘Baskarp’ sand, the sand used in the hydraulic fracturing experiments at GeoDelft. The material parameters for this sand are obtained from triaxial tests.

Finally, the influence of confining stress on the biaxial test simulation results is investigated to find out for which stress range a given set of parameters still gives a realistic behaviour.

An important aspect in all simulations is the interpretation of the results. Since the discrete element code used is two-dimensional, what happens in the third dimension is not known and results could be interpreted assuming either a plane-strain or a plane-stress situation. Both situations are discussed and compared.
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1 Introduction

In this report, biaxial tests are simulated with the two-dimensional discrete element code PFC2D from Itasca. The simulations are similar to those in [Baars 1996]. However, a different discrete element method, based on static equilibrium, was used there while the PFC2D code is a dynamic analysis.

The calculations are made for non-cohesive materials. Therefore, the behaviour of the particles does not include bonding. The main objective of the calculations is to determine which micro parameters should be chosen to achieve a certain macro-behaviour. To understand the influence of certain micro parameters first some simulations are made to see if the change in one of the micro-parameters has a major effect on all of the macro-parameters (stiffness, poisson’s ratio, angle of internal friction and the angle of dilatancy) or of just one.

When the influence of each micro parameter is known, this knowledge is applied to adjust the micro parameters in such a way that the macro parameters resulting from the biaxial test simulation are similar to those of Swedish ‘Baskarp’ sand. The material parameters for this sand are obtained from triaxial tests. Dependence of the stiffness of the modelled material on the confining stress is also investigated to see if the results are realistic for a wide stress range.

An important aspect is the interpretation of the results. Since the discrete element code used is two-dimensional, what happens in the third dimension is not known and results could be interpreted assuming either a plane-strain or a plane-stress situation. Both situations are discussed and compared.

Chapter 2 gives the difference between the plane-strain and plane-stress situation, Chapter 3 discusses the set-up of the biaxial test simulations and the modelling of the Swedish ‘Baskarp’ sand with the non-linear Hertz contact model and the linear contact model. Chapter 4 discusses the influence of confining stress on the results of biaxial test simulations for both contact models. Conclusions are presented in Chapter 5.
2 Plane-strain versus plane-stress behaviour

The program PFC2D used for the biaxial test simulations is a two-dimensional discrete element code. Contrary to finite element programs where, for example, the stress in the third dimension can be calculated in case of a plane-strain situation, it is not known what happens in the third dimension in this case. The third dimension is simply left out and no stress or strain can be prescribed in that direction. The macro-behaviour that results from the simulations, however, can only be compared to the three-dimensional macro parameters that we commonly understand.

Therefore, in this chapter the two extremes of plane-stress and plane-strain are described and for both situations, the macro parameters will be compared, in order to view the differences between both interpretations.

2.1 Linear elastic behaviour

It is assumed that in the beginning of a biaxial test the material behaves according to Hook’s linear elastic relation between stresses and strains. In principal stress space the behaviour is as follows:

\[
\begin{bmatrix}
\dot{\sigma}_1 \\
\dot{\sigma}_2 \\
\dot{\sigma}_3
\end{bmatrix} = \frac{1}{E} \begin{bmatrix}
1 & -\nu & -\nu \\
-\nu & 1 & -\nu \\
-\nu & -\nu & 1
\end{bmatrix} \begin{bmatrix}
\dot{\varepsilon}_1 \\
\dot{\varepsilon}_2 \\
\dot{\varepsilon}_3
\end{bmatrix}
\] (2.1)

Here, \( \varepsilon_i \) and \( \sigma_i \) \((i=1,2,3)\) are the strain and stress rates in the principal directions, \( E \) is the Young’s modulus and \( \nu \) is poisson’s ratio. In case of a biaxial test the principal directions are normal to the walls of the cell. Suppose that when viewed two-dimensionally the third principal direction corresponds to the out-of plane direction. Then for a plane-strain situation \( \varepsilon_3 = 0, \dot{\varepsilon}_3 = 0 \) and in case of plane-stress \( \sigma_3 = 0, \dot{\sigma}_3 = 0 \).

In case of plane-strain, the stress in the third direction can be calculated from the third equation of (2.1):

\[
\dot{\sigma}_3 = \nu (\dot{\sigma}_1 + \dot{\sigma}_2)
\] (2.2)

Substituting this in (2.1) gives:

\[
\begin{bmatrix}
\dot{\sigma}_1 \\
\dot{\sigma}_2 \\
\dot{\sigma}_3
\end{bmatrix} = \frac{1}{E} \begin{bmatrix}
1 - \nu^2 & -\nu (1+\nu) \\
-\nu (1+\nu) & 1 - \nu^2
\end{bmatrix} \begin{bmatrix}
\dot{\varepsilon}_1 \\
\dot{\varepsilon}_2
\end{bmatrix}
\] (2.3)

For the plane-stress situation, with the third equation of (2.1), the strain in the third direction can be calculated from

\[
\dot{\varepsilon}_3 = -\frac{\nu}{E} (\dot{\varepsilon}_1 + \dot{\varepsilon}_2)
\] (2.4)
The relation between strain and stress rates follows directly from (2.1):

\[
\begin{bmatrix}
\frac{\varepsilon_1}{E} \\
\frac{\varepsilon_2}{E}
\end{bmatrix} = \frac{1}{E} \begin{bmatrix}
1 & -\nu \\
-\nu & 1
\end{bmatrix} \begin{bmatrix}
\sigma_1 \\
\sigma_2
\end{bmatrix}
\]  \hspace{1cm} (2.5)

Let the axial direction in the biaxial test be the 1-direction. In the test first a stress state is made where \(\sigma_1 = \sigma_2 = \sigma_c\) is the confining stress. Then during the actual test, the axial stress is increased while keeping \(\sigma_2\) constant. During this process \(\sigma_2 = 0\) and the axial strain rate can be expressed in the axial stress rate for both the plane strain and plane stress situations with equations (2.3) and (2.5). From this, the Youngs modulus \(E\) can be expressed in terms of the ratio \(\sigma_1/\varepsilon_1\), a quantity that can be directly read from the actual calculation results. The Young’s modulus for the plane strain situation is:

\[
E = (1 - \nu^2) \frac{\varepsilon_1}{\varepsilon_1} \hspace{1cm} (2.6)
\]

And the Young’s modulus for the plane stress situation becomes:

\[
E = \frac{\varepsilon_1}{\varepsilon_1} \hspace{1cm} (2.7)
\]

Which is equal to the slope of the curve in the \(\sigma_1-\varepsilon_1\) diagram. It can be seen that when poisson’s ratio is zero, the Young’s modulus is equal for the plane-stress and plane strain situations. And in case of the for normal materials maximum value \(\nu = 0.5\) this means that the maximum deviation between both results is 25%.

The poisson’s ratio can be obtained by determining the slope of the volumetric strain versus the axial strain curve. Since the program is two-dimensional, the volumetric strain is defined as: \(\varepsilon_{vol} = \varepsilon_1 + \varepsilon_2\). For the plane-strain situation the volumetric strain rate can be expressed in terms of the axial stress rate, with equation 2.3 setting \(\sigma_2 = 0\):

\[
\varepsilon_{vol} = \varepsilon_1 + \varepsilon_2 = \frac{1}{E} (1 - \nu - 2\nu^2) \varepsilon_1 \hspace{1cm} (2.8)
\]

Using equation (2.6), \(\sigma_1\) can be expressed in terms of \(\varepsilon_1\) and the ratio between the volumetric strain rate and axial strain rate becomes:

\[
\frac{\varepsilon_{vol}}{\varepsilon_1} = \frac{1 - 2\nu}{1 - \nu} \hspace{1cm} (2.9)
\]

For the plane-stress situation, from equation (2.5) it can be directly observed that:

\[
\varepsilon_1 = -\nu \varepsilon_2 \hspace{1cm} (2.10)
\]

And from this it follows that:

\[
\frac{\varepsilon_{vol}}{\varepsilon_1} = 1 - \nu \hspace{1cm} (2.11)
\]
So when the slope is determined the value of the poisson’s ratio can be calculated for both situations. The differences between the plane stress and plane strain situations for the poisson’s ratio are not as directly seen as for the elastic stiffness case. However, some things can be visualised, see Table 2.1:

Table 2.1 Values of the poisson's ratio for the plane strain and plane stress situations for different slopes of the Volumetric strain versus axial strain curve

<table>
<thead>
<tr>
<th>Slope Vol. strain/Axial strain</th>
<th>( \nu ) (plane strain)</th>
<th>( \nu ) (plane stress)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.5</td>
<td>1</td>
</tr>
<tr>
<td>0.5</td>
<td>0.3</td>
<td>0.5</td>
</tr>
<tr>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

It can be seen that when the slope has such values that the poisson’s ratio for the plane strain case has realistic values between 0 and 0.5. The poisson’s ratio for the plane stress situation has unrealistic values larger than 0.5. Test calculations have to show if such a phenomenon occurs.

A description of how to determine the slopes of the \( \sigma_1 - \varepsilon_1 \) and \( \varepsilon_{vol} - \varepsilon_1 \) curves for a simulated biaxial test is discussed in the next chapter.

### 2.2 Angle of internal friction and dilatancy angle

A linear elastic and ideal plastic material model is assumed with a Mohr-Coulomb yield function. Then the angle of internal friction \( \varphi \) and the cohesion \( c \) are the parameters to be determined from the simulated biaxial tests. There are six yield functions in the principal stress space, but for the biaxial test only two are relevant:

\[
\begin{align*}
  f_1 &= \frac{1}{2} (\sigma_1 - \sigma_2) - \frac{1}{2} (\sigma_1 + \sigma_2) \sin \varphi - c \cos \varphi & \sigma_2 \leq \sigma_3 \leq \sigma_1 \\
  f_2 &= \frac{1}{2} (\sigma_1 - \sigma_3) - \frac{1}{2} (\sigma_1 + \sigma_3) \sin \varphi - c \cos \varphi & \sigma_3 \leq \sigma_2 \leq \sigma_1
\end{align*}
\] (2.12)

These are valid when the stress is positive in case of pressure. If the behaviour is elastic all of the functions are negative, in case of plasticity, one or two functions are zero. Here we look at non-cohesive materials, so \( c = 0 \).

Also, a plastic flow rule is assumed according to:

\[
\varepsilon_p = \lambda \frac{\partial g_1}{\partial \sigma}
\] (2.13)

With plastic potential functions:

\[
\begin{align*}
  g_1 &= (\sigma_1 - \sigma_2) - (\sigma_1 + \sigma_2) \sin \psi \\
  g_2 &= (\sigma_1 - \sigma_3) - (\sigma_1 + \sigma_3) \sin \psi
\end{align*}
\] (2.14)
where $\psi$ is the angle of dilatancy. Plastic flow occurs when either $f_1$ or $f_2$ becomes zero this happens when:

$$\frac{\sigma_1}{\sigma_2} = \frac{1 + \sin \phi}{1 - \sin \phi}$$  \hspace{1cm} (2.15)

for $f_1$ and when:

$$\frac{\sigma_1}{\sigma_3} = \frac{1 + \sin \phi}{1 - \sin \phi}$$  \hspace{1cm} (2.16)

for $f_2$.

In case of the plane stress interpretation, $\sigma_3=0$ it is observed that $f_2 > 0$. This is not possible, therefore it would be impossible to reach the initial stress state. The only plane stress interpretation one could make, is to assume $\sigma_3=\sigma_2$ and both stress rates are zero, then $f_2$ would become zero at the same moment as $f_1$.

For the plane strain situation, in the beginning of the test, $\sigma_3$ is smaller than $\sigma_2$, during this stage it’s possible for $f_2$ to become active, depending on the angle of internal friction $\phi$, see equation (2.16). When $\sigma_1$ reaches the value of $\sigma_2 (1-\nu)/\nu$, $\sigma_3$ becomes equal to $\sigma_2$. If by this point $f_2$ wasn’t zero, it will not become zero because now $f_1$ will first become zero and when this happens the sample collapses while $\sigma_1$ remains constant. If $f_2$ does become zero initially, a flow mechanism occurs where there is plastic flow in the 3-direction. Because the total strain in that direction is zero there must be an elastic strain in the 3-direction. So the stress $\sigma_1$ can continue to be build up be it with a reduced sample stiffness. When flow function $f_1$ finally becomes active, using the flow rule and plastic potential function $g_1$, the plastic strain can be calculated:

$$g_\tau = \lambda \begin{bmatrix} 1 - \sin \psi \\ -1 - \sin \psi \\ 0 \end{bmatrix}$$  \hspace{1cm} (2.17)

Since $\sigma_2$ is constant, the stress $\sigma_1$ also has to remain constant to satisfy $f_1=0$. If $f_2$ had been active it will stop because plastic straining can only occur for that mechanism if elastic straining in the 3-direction is possible because the total strain in that direction has to be zero. Therefore, once $f_1$ becomes active, there is only plastic flow according to (2.17). Then the slope of the volumetric strain versus axial strain curve will be:

$$\frac{g_\tau_{vol}}{g_\tau} = \frac{-2 \sin \psi}{1 - \sin \psi}$$  \hspace{1cm} (2.18)
Note that when using a plane stress situation and having $\sigma_3 = \sigma_2$, both plastic flow functions would be active. Now, the plastic strain rate is the sum of (2.17) and a similar equation using $g_2$ and the same value $\lambda$ because of symmetry of the 2 and 3 directions:

$$
\dot{\varepsilon} = \lambda \begin{bmatrix}
1 - \sin \psi \\
-1 - \sin \psi \\
0
\end{bmatrix} + \lambda \begin{bmatrix}
1 - \sin \psi \\
0 \\
-1 - \sin \psi
\end{bmatrix}
$$

(2.19)

Because $\varepsilon_{vol} = \varepsilon_1 + \varepsilon_2$, the slope of the volumetric strain versus axial strain curve becomes:

$$
\frac{\varepsilon_{vol}}{\dot{\varepsilon}_x} = \frac{1 - 3 \sin \psi}{2 - 2 \sin \psi}
$$

(2.20)

This expression seems strange because when $\psi = 0$, the slope of the curve is $\frac{1}{2}$. Tests have to determine if this phenomenon is indeed seen for the two-dimensional biaxial test simulations.

### 2.3 Macro parameters from a triaxial test

The macro parameters resulting from a biaxial test simulation will be compared to the results from an actual triaxial test. For a triaxial test $\sigma_3 = \sigma_2 = \text{constant}$ and it follows directly from (2.1) that

$$
E = \frac{\dot{\varepsilon}_x}{\dot{\varepsilon}_x}
$$

(2.21)

Also from (2.1) it can be seen that:

$$
\frac{\varepsilon_{vol}}{\dot{\varepsilon}_x} = 1 - 2\nu
$$

(2.22)

For plasticity both of the flow functions (2.12) become active at the same time resulting in an angle of internal friction according to the peak stress:

$$
\left(\frac{\sigma_1}{\sigma_3}\right)_{\text{max}} = \frac{1 + \sin \varphi}{1 - \sin \varphi}
$$

(2.23)

During plastic flow, using the flow rule, the strain can be described with (2.19). However, this time the volumetric strain is the sum of the strains in all three directions. This results in:

$$
\frac{\varepsilon_{vol}}{\dot{\varepsilon}_x} = \frac{-2 \sin \psi}{1 - \sin \psi}
$$

(2.24)

which is the same as equation (2.18).
2.4 Conclusions

The differences between the plane strain and plane stress situation have been calculated assuming a linear elastic and ideal plastic material. The difference in elastic stiffness has shown to be at most 25%. For poisson’s ratio and the angle of dilatancy, it’s possible to see unrealistic results during the calculations in case of the plane stress interpretation. In the next chapter, a test calculation is made to see if such a phenomenon occurs and to decide which interpretation is more realistic and will be adopted for further studies.
3 Description of the biaxial test simulations

In this chapter, first the set up of a biaxial test in the discrete element program PFC2D is described and the method of determining the macro parameters from the simulations is discussed. Then simulations are made by adjusting certain micro parameters and observing the effect on the macro parameters to find some general trends that could be used for creating a material with certain characteristics. These ideas are then used to find suitable micro parameters to model a Swedish sand called Baskarp sand for which two triaxial test results were available.

3.1 Set up of biaxial test simulations

To model a biaxial test in the program PFC2D, first a sample has to be created. In PFC2D, a linear or a non-linear Hertz-Mindlin contact model can be used for the contact behaviour between the particles. For the current investigation, the non-linear Hertz-Mindlin contact model has been used. For this contact model two micro parameters must be given, namely a shear stiffness $G_m$ and a poisson’s ratio $\nu_m$. Here the subscript $m$ denotes micro parameters. Note that this shear stiffness and poisson’s ratio have no direct connection to those parameters on macro scale. Further, for the particles a friction coefficient $\text{fric}$ can be given which determines which fraction of the normal force the particle-particle contact can take as shear force before sliding occurs. Then, the particles have a certain radius. A minimum and maximum radius $r_{\text{min}}$ and $r_{\text{max}}$ can be given and a uniform or Gaussian radius distribution can be chosen. Particles are randomly generated in PFC with radii between minimum and maximum radius according to the given distribution.

The simulations are performed with $N$ particles and a uniform radius distribution. The average particle radius is $r_{\text{av}} = (r_{\text{min}} + r_{\text{max}})/2$. $N$ particles have a total surface of $A = N \pi r_{\text{av}}^2$. To create a sample with a certain porosity $n$, the cell size has to be $A_{\text{cel}} = A/(1-n)$. For the cell, the height is chosen to be 2.5 times the width, so when $A_{\text{cel}}$ is known, the cell dimensions are fixed.

The simulations are made with 1000 particles. The minimum particle radius $r_{\text{min}} = 0.04$ cm and the maximum radius $r_{\text{max}} = 0.16$ cm. With a porosity of 0.12, the cell dimensions are 9.45x3.77 cm. First the walls (cell boundaries) are created and their position is kept fixed. Then, the particles are put in the cell but with a reduced radius. Later, the radius is expanded to the input radius. In the next step the walls are no longer fixed, but an external initial stress is applied, $\sigma_1 = \sigma_2 = \sigma_{\text{init}}$, to create an isotropic stress state. During this entire process the internal friction is set to a relatively low value. After applying the initial stress, the internal friction coefficient, $\text{fric}$, is set to the desired value. Then, the biaxial test is performed by changing the boundary conditions. The upper and lower walls of the sample are given a prescribed velocity in vertical direction to achieve compression of the sample while the stress on the left and right walls is kept constant at the initial stress value, see Figure 3.1.
3.2 Determining the macro parameters from the Biaxial test simulations

The simulations of the biaxial tests are made with certain values for the micro parameters. The macroscopic quantities that result from the test or are applied as boundary conditions, are the two stresses in directions perpendicular to the cell walls \( \sigma_1 \) and \( \sigma_2 \) and the two strains \( \varepsilon_1 \) and \( \varepsilon_2 \). When the micro parameters are adjusted, the effect on the macro scale is measured by observing these quantities. From these quantities, the macro parameters are determined using the theory discussed in the previous chapter.

Two plots were made of the results, the deviatoric stress \( (\sigma_1 - \sigma_2) \) versus the axial strain and the negative volumetric strain versus the axial strain. An example of a calculation is given in Figure 3.2 and Figure 3.3. The results do not follow an exact elastic-ideal plastic behaviour like in finite element calculations. The behaviour looks more like that of triaxial test results with real materials having a stiffness decreasing slowly until a peak stress is reached. For this reason, it has been chosen to determine the elastic parameters \( E_{50} \) and \( v_{sv} \) like in triaxial tests.
The method for calculating the macro parameters is automated in a computer program, which first reads the data from both curves. From Figure 3.2, first the maximum deviatoric stress is determined, which in this case is 302 kPa. Then the curve is followed again until half of this value is reached (151 kPa) and the axial strain in this point is found to be 0.219%. A line is drawn through the origin and this point. The slope of this line is then used to determine the stiffness according to a plane strain or plane stress interpretation. To determine poisson’s ratio, Figure 3.3 is followed until the previously determined axial strain (at half maximum deviatoric stress) is reached. Then a line is drawn through the origin and this point, the slope of which is used to determine poisson’s ratio following a plane strain or plane stress interpretation.

The angle of internal friction is calculated using the maximum value of the deviatoric stress. Because the stress $\sigma_2$ is known, the maximum $\sigma_1/\sigma_2$ can be calculated and with equation (2.15) the angle of internal friction can be calculated. The angle of dilatancy is calculated from the slope of the
volumetric- versus axial strain curve in the plastic regime. Here it is assumed that the behaviour is fully plastic when the curve passes through zero again, see Figure 3.3. From this point until the final calculation step, a least squares method is used to determine the line best fitting the data. This line is also shown in Figure 3.3. From the slope, the angle can be determined according to either plane strain or plane stress interpretation by using equations (2.18) and (2.20). It may be possible that the curve stays below zero, in this case the starting point of the least squares method is chosen two times the axial strain at half maximum deviatoric stress.

The biaxial test simulation presented in the previous figures was made with parameters shear stiffness $G_m=10\text{GPa}$, poisson’s ratio $\nu_m=0.16$ and friction coefficient $fric=0.8$. The macro parameters resulting from the test are given in Table 3.1:

Table 3.1 Differences between plane strain and plane stress interpretation.

<table>
<thead>
<tr>
<th></th>
<th>plane strain interpretation</th>
<th>plane stress interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{50}$ [MPa]</td>
<td>59.3</td>
<td>65.7</td>
</tr>
<tr>
<td>$\nu_{50}$</td>
<td>0.31</td>
<td>0.45</td>
</tr>
<tr>
<td>friction angle $\varphi$ [degrees]</td>
<td>35.7</td>
<td>35.7</td>
</tr>
<tr>
<td>dilatancy angle $\psi$ [degrees]</td>
<td>16.8</td>
<td>34.6</td>
</tr>
</tbody>
</table>

The elastic stiffness is nearly the same as was concluded in the theory. However, poisson’s ratio is very high for the plane stress interpretation and the dilatancy angle is also very large. For this reason it has been chosen to adapt the plane strain interpretation of the biaxial test results. Accordingly, this interpretation will be used in the following sections.

### 3.3 Effect of micro parameters on the macro parameters

With the set up as described in section 3.1, the three micro parameters: shear stiffness $G_m$, poisson’s ratio $\nu_m$ and friction coefficient $fric$ are varied to observe the effect on a macro scale. The initial stress is set to 1 bar.

In the first series of calculations the shear stiffness was taken $G_m=10\text{GPa}$ and for the poisson’s ratio $\nu_m=0.16$. The internal friction was varied. The results are shown in Figure 3.5 and Figure 3.6. For an increasing friction coefficient the peak stress becomes larger and therefore the angle of internal friction also becomes larger. The angle of dilatancy also is larger for increasing friction and is approximately zero for $fric=0.0$. The macro parameters determined from these biaxial test simulations are summed up in Table 3.2. The largest variation is in the dilatancy angle and angle of internal friction. The stiffness $E_{50}$ also increases a little for increasing friction coefficients. These results were also found by [Baars 1996].

Table 3.2 Macro parameters for biaxial test simulations with different friction coefficients.

<table>
<thead>
<tr>
<th></th>
<th>fric=0.0</th>
<th>fric=0.2</th>
<th>fric=0.4</th>
<th>fric=0.6</th>
<th>fric=0.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{50}$ [MPa]</td>
<td>41.5</td>
<td>38.8</td>
<td>48.8</td>
<td>55.9</td>
<td>59.3</td>
</tr>
<tr>
<td>$\nu_{50}$</td>
<td>0.29</td>
<td>0.37</td>
<td>0.34</td>
<td>0.32</td>
<td>0.31</td>
</tr>
<tr>
<td>friction angle $\varphi$</td>
<td>20.3</td>
<td>23.6</td>
<td>29.6</td>
<td>32.7</td>
<td>35.7</td>
</tr>
<tr>
<td>dilatancy angle $\psi$</td>
<td>-0.6</td>
<td>6.6</td>
<td>11.3</td>
<td>14.1</td>
<td>16.8</td>
</tr>
</tbody>
</table>
Figure 3.5 Deviatoric stress versus axial strain for various friction coefficients.

Figure 3.6 Volumetric strain versus axial strain for various friction coefficients.

The second series of simulations are performed for a varying shear stiffness $G_m$. The friction coefficient is now kept constant at $fric=0.8$. The results are presented in Table 3.3 and Figure 3.7 and Figure 3.8:

Table 3.3 Macro parameters resulting from biaxial test with varying (micro) shear stiffness.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$G_m=1$GPa</th>
<th>$G_m=2$GPa</th>
<th>$G_m=4$GPa</th>
<th>$G_m=10$GPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{30}$ [MPa]</td>
<td>14.8</td>
<td>23.4</td>
<td>32.9</td>
<td>59.3</td>
</tr>
<tr>
<td>$v_{30}$</td>
<td>0.27</td>
<td>0.28</td>
<td>0.31</td>
<td>0.31</td>
</tr>
<tr>
<td>friction angle $\varphi$</td>
<td>32.6</td>
<td>34.4</td>
<td>34.4</td>
<td>35.7</td>
</tr>
</tbody>
</table>
For increasing micro shear stiffness, the elastic stiffness $E_{50}$ increases significantly. Also, the angle of internal friction increases, but only slightly. Poisson’s ratio remains almost constant.

The last micro parameter to be varied is the microscopic Poisson’s ratio $\nu_m$. This is done with a shear stiffness $G_m=10\,\text{GPa}$ and a friction coefficient $\text{fric}=0.8$. The results are presented in Table 3.4, Figure 3.9 and Figure 3.10. Here it can be seen that varying the microscopic Poisson’s ratio has very little effect on the macro parameters. The elastic stiffness increases slightly for increasing $\nu_m$, but not significantly. These results were also found by [Baars 1996].
For each of the three micro parameters $G_m$, $\nu_m$ and $fric$, their effects on the macro scale have been described. The results suggest that a material with a certain elastic stiffness and angle of internal friction could be produced by adjusting the micro parameters. However, the discussed micro parameters have no effect on the poisson’s ratio and also the angle of dilatancy is strongly linked to the angle of internal friction. This means that a certain value of the internal friction could be achieved by adjusting the friction coefficient $fric$ and then the desired elastic stiffness could be reached by adjusting the micro shear stiffness $G_m$. The angle of dilatancy is a result of this process and poisson’s ratio cannot be changed also.

Table 3.4 Results of biaxial test simulations with varying (micro) poisson’s ratio.

<table>
<thead>
<tr>
<th></th>
<th>$\nu_m=0.0$</th>
<th>$\nu_m=0.16$</th>
<th>$\nu_m=0.30$</th>
<th>$\nu_m=0.45$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{50}$ [MPa]</td>
<td>50.9</td>
<td>59.3</td>
<td>63.6</td>
<td>73.2</td>
</tr>
<tr>
<td>$\nu_{50}$</td>
<td>0.33</td>
<td>0.31</td>
<td>0.31</td>
<td>0.33</td>
</tr>
<tr>
<td>friction angle $\varphi$</td>
<td>36.1</td>
<td>35.7</td>
<td>36.4</td>
<td>36.4</td>
</tr>
<tr>
<td>dilatancy angle $\psi$</td>
<td>16.9</td>
<td>16.8</td>
<td>16.6</td>
<td>16.6</td>
</tr>
</tbody>
</table>

Figure 3.9 Deviatoric stress versus axial strain for varying poisson's ratio
Figure 3.10 Volumetric strain versus axial strain for varying poisson's ratio

3.4 Fitting of triaxial test results for Swedish ‘Baskarp’ sand

Two triaxial tests were performed on the Swedish ‘Baskarp’ sand for a cell stress of approximately 164 kPa. The material parameters resulting from the two tests are given in Table 3.5. The tests itself are presented in Appendix 1. These tests were performed after cyclic tests, which may have some influence on the strength parameters, however, currently these were the only available triaxial tests for Swedish ‘Baskarp’ sand.

Table 3.5 Material parameters derived from triaxial tests

<table>
<thead>
<tr>
<th>parameter</th>
<th>Test 1</th>
<th>Test 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus $E_{50}$ [MPa]</td>
<td>186.33</td>
<td>157.84</td>
</tr>
<tr>
<td>Friction angle $\varphi$ [°]</td>
<td>42.78</td>
<td>40.94</td>
</tr>
<tr>
<td>angle of dilatancy $\psi$ [°]</td>
<td>19.02</td>
<td>14.86</td>
</tr>
</tbody>
</table>

The cohesion is zero because it’s sand. The poisson’s ratio is difficult to determine from the tests. Biaxial tests are simulated and interpreted according to a plane-strain situation. As seen from previous tests, it’s possible to choose the micro parameters in such a way that the stiffness and friction angle are in accordance with tests. The stiffness and friction angle should be equal to the average value from the two triaxial tests. The poisson’s ratio and angle of dilatancy are difficult to fit.

The biaxial test simulations were made with 1000 particles and a porosity of 0.12. The cell height was 2.5 times the cell width and the maximum radius of the particles is four times the minimum radius. As average radius a value of 0.1 is chosen. With this the size of the cell is known. Calculations were made using the Hertz-Mindlin contact model as in previous simulations. During the tests the micro parameters for the shear stiffness in the Hertz-Mindlin model $G_m$ and internal friction coefficient $\text{fric}$ were adjusted to match the experimental result. The initial stress-state was created setting the internal friction $\text{fric}=0.05$. Then for the actual test the friction was set to different values. The set of parameters that gave the best results is given in Table 3.6. Note that the micro shear modulus $G_m$ has a value of 39GPa. The measured shear modulus value for quartz is 34GPa according to the Handbook of Physics and Chemistry, so the obtained value seems realistic.
Table 3.6 Parameters for best simulation of Swedish 'Baskarp' sand

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>shear modulus $G_m$ [GPa]</td>
<td>39</td>
</tr>
<tr>
<td>poisson’s ratio $\nu_m$</td>
<td>0.16</td>
</tr>
<tr>
<td>friction coefficient during biaxial test $\text{fric}$</td>
<td>1.3</td>
</tr>
<tr>
<td>friction during assembly and applying initial stress state</td>
<td>0.05</td>
</tr>
<tr>
<td>porosity $n$</td>
<td>0.12</td>
</tr>
<tr>
<td>maximum radius/minimum radius</td>
<td>4</td>
</tr>
</tbody>
</table>

The results of the calculation with the above parameters are given in the next figures:

Figure 3.11 Deviatoric stress versus axial strain curve for the Swedish 'Baskarp' sand simulation

Figure 3.12 Volumetric strain versus axial strain for the Swedish ‘Baskarp’ sand simulation

The Young’s modulus $E_{50}$ and friction angle corresponding with the maximum deviatoric stress is calculated from Figure 3.11 with the post processing program. Poisson’s ratio and the angle of dilatancy are calculated from Figure 3.12. These parameters are given in Table 3.7. The Young’s modulus and friction angle correspond well with the average from the two triaxial tests. Poisson’s
ratio of 0.33 is also a common value for sands. The angle of dilatancy is a little higher than the average from the tests but not very far off.

Table 3.7 Macro parameters resulting from biaxial test with 1000 particles

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus $E_{50}$ [MPa]</td>
<td>173</td>
</tr>
<tr>
<td>poisson’s ratio $v_{50}$</td>
<td>0.33</td>
</tr>
<tr>
<td>Friction angle $\phi$ [°]</td>
<td>40.9</td>
</tr>
<tr>
<td>angle of dilatancy $\psi$ [°]</td>
<td>20.5</td>
</tr>
</tbody>
</table>

Two extra simulations were performed using the same micro parameters only now with 2000 and 4000 particles in order to investigate the deviation in resulting macro parameters. The deviatoric stress versus axial strain and volumetric- versus axial strain curves look very similar. The resulting macro parameters are displayed in Table 3.8. The Young’s modulus increases a little, but the friction angle and angle of dilatancy remain almost constant.

Table 3.8 Macro parameters resulting from biaxial tests with 2000 and 4000 particles

<table>
<thead>
<tr>
<th>Parameter</th>
<th>2000 particle test</th>
<th>4000 particle test</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus $E_{50}$ [MPa]</td>
<td>206</td>
<td>216</td>
</tr>
<tr>
<td>poisson’s ratio $v_{50}$</td>
<td>0.30</td>
<td>0.26</td>
</tr>
<tr>
<td>Friction angle $\phi$ [°]</td>
<td>42.6</td>
<td>41.0</td>
</tr>
<tr>
<td>angle of dilatancy $\psi$ [°]</td>
<td>21.8</td>
<td>22.0</td>
</tr>
</tbody>
</table>

3.5 Linear contact model parameters

In PFC2D also simulations can be performed with a linear contact model. Then it is as having two linear springs in a contact between particles, one for the normal stiffness given by the constant $k_n$ and one for the shear stiffness given by $k_s$. The normal force is proportional to the normal stiffness and the overlap of two particles. The shear force is proportional to the shear stiffness and the relative rotation between two particles. The friction coefficient is the same as in the Hertz model parameters and having the same influence on the macro parameters. The normal contact stiffness has direct influence on the Young’s modulus while the ratio of $k_n/k_s$ has some influence on the poisson ratio (see PFC2D manual). After varying some parameters, a good agreement with the ‘Baskarp’ sand characteristics was found with parameters as presented in Table 3.9. The simulation results are given in Table 3.10.

Table 3.9 :Best fit parameters for ‘Baskarp’ sand with the linear contact model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>contact normal stiffness $k_n$ [Pa]</td>
<td>900E6</td>
</tr>
<tr>
<td>contact shear stiffness $k_s$ [Pa]</td>
<td>400E6</td>
</tr>
<tr>
<td>friction coefficient during biaxial test $fric$</td>
<td>0.9</td>
</tr>
<tr>
<td>friction during assembly and applying initial stress state</td>
<td>0.05</td>
</tr>
<tr>
<td>porosity $n$</td>
<td>0.12</td>
</tr>
<tr>
<td>maximum radius/minimum radius</td>
<td>4</td>
</tr>
</tbody>
</table>
Table 3.10 Macro parameters resulting from biaxial test with linear contact model and 1000 particles.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus $E_{50}$ [MPa]</td>
<td>193</td>
</tr>
<tr>
<td>poisson’s ratio $\nu_{50}$</td>
<td>0.36</td>
</tr>
<tr>
<td>Friction angle $\phi$ [°]</td>
<td>40.9</td>
</tr>
<tr>
<td>angle of dilatancy $\psi$ [°]</td>
<td>16.8</td>
</tr>
</tbody>
</table>

3.6 Influence of particle size distribution

Previous simulations were all made with a uniform particle size distribution with a maximum radius/minimum radius ratio of 4:1. Three additional biaxial test simulations were made with 1000 particles and a uniform particle size distribution with $r_{min}/r_{max}$ ratio’s of 2:1, 4:3 and 1.05:1. The results are given in Table 3.11.

Table 3.11 : Biaxial test results as a function of the ratio of maximum particle radius to minimum particle radius.

<table>
<thead>
<tr>
<th>parameter</th>
<th>4:1</th>
<th>2:1</th>
<th>4:3</th>
<th>1.05:1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus $E_{50}$ [MPa]</td>
<td>173</td>
<td>184</td>
<td>181</td>
<td>68.6</td>
</tr>
<tr>
<td>poisson’s ratio $\nu_{50}$</td>
<td>0.33</td>
<td>0.3</td>
<td>0.29</td>
<td>0.52</td>
</tr>
<tr>
<td>Friction angle $\phi$ [°]</td>
<td>40.9</td>
<td>39.3</td>
<td>40.6</td>
<td>51.0</td>
</tr>
<tr>
<td>angle of dilatancy $\psi$ [°]</td>
<td>20.5</td>
<td>16.9</td>
<td>16.6</td>
<td>21.4</td>
</tr>
</tbody>
</table>

There is not a great deal of difference between the ratio’s 4:1, 2:1 and 4:3, the variations could be due to the random particle generation and not so much due to the size distribution. The results for the 1.05:1 ratio, however are much different. There is a much lower Young’s modulus, an extremely high friction angle and a poisson’s ratio of more than 0.5! Probably these results are caused by the particles having nearly the same radius, this creates a kind of regular lattice structure (particles tend to go to a hexagonal packing if their size is equal).

It is therefore preferred not to use ratio’s close to 1:1. The ratio of 4:3 gives still good results but lower ratio’s will give strange results at a given point.
4  Biaxial test simulations for different confining stresses

In the previous Chapter, it has been shown that the Swedish ‘Baskarp’ sand used in the hydraulic fracturing experiments could be modelled well in PFC2D with both the linear contact model and the non-linear Hertz-Mindlin model. However, the fit was made for a confining stress of 164 kPa only, since at this stress there were triaxial test results. Because the sand will be used in a wide stress range in future hydraulic fracturing experiments, here the behaviour of material modelled with PFC2D will be investigated for a wide stress range from 2 bar to 100 bar. Although we currently have no data on the ‘Baskarp’ sand at high confining stress, it’s known from the literature that the stiffness of sand increases significantly with increasing confining stress for such a large stress interval. Such behaviour should also be present in the PFC2D simulations as well if anything is to be said about the behaviour under various stresses during hydraulic fracturing simulations for example.

To test this, a number of biaxial test simulations has been performed to observe the increase of stiffness with confining stress. Simulations were made for the linear contact model and for the non-linear Hertz contact model. The used micro parameters for the particles are the best fit parameters for the Swedish ‘Baskarp’ sand as described in the previous chapter. The sample with applied confining stress as initial stress state has been generated in the same way as described earlier.

The biaxial test simulations were performed for confining stresses of 2, 4, 10, 20, 40 and 100 bar. For each situation, the Young’s modulus has been calculated. The results are shown in Figure 4.1.

![Figure 4.1: Young's modulus as a function of confining stress for the linear contact model and the non-linear Hertz contact model compared with a power law formula.](image)

The figure shows that the non-linear Hertz contact model increases significantly with confining stress while the results for the linear contact model show only a slight increase. This was expected because the stiffness of each contact in the linear model is a constant. With increased confining stress, the...
sample is compressed and slightly more contacts are created in the sample. This somewhat greater “contact-density” results in a slight increase of stiffness. The Hertz model on the contrary has a non-linear stiffness for contacts with increasing displacement, hence the significant increase in stiffness.

Also shown in Figure 4.1 is a power law function of the following form:

\[ E = E_{ref} \left( \frac{p}{p_{ref}} \right)^n \]  

(4.1)

In the literature such a power law is often used to describe the increase in shear modulus \( G \) with isotropic stress \( p \). If it’s assumed that the poisson’s ratio remains constant then the same formula applies for the Young’s modulus as well. In Figure 4.1, the reference values are \( p_{ref} = 2 \) bar and \( E_{ref} \) is the Young’s modulus at 2 bar confining stress resulting from the simulation at 2 bar. The power law formula was drawn for \( n = 0.4 \). For sands in the stress range common in soil mechanics normally \( n = 0.5 \) is used, but for higher stresses used in rock mechanics the value 0.3 is used. Therefore the value 0.4 seems realistic. The presentation of the power law formula is just to estimate the increase of Young’s modulus with confining stress and is not intended to be an exact match of measurements.

The Hertz model agrees reasonably well with the given power-law formula results for \( n = 0.4 \) and the model seems quite realistic for sand type materials. Therefore, the Hertz model is preferred if a larger stress range is needed in simulations. The linear model can be used successfully only when the contact stiffness is matched to the confining stress for a particular stress state to obtain the desired stiffness of the sample. The realistic value of \( n = 0.4 \) also indicates that the increase in stiffness is slower than the increase in confining stress. Therefore at higher stress, the sample is relatively softer.
5 Conclusions

- For each of the three micro parameters $G_m$, $\nu_m$ and $fric$, their effects on the macro scale have been determined. The results suggest that a material with a certain elastic stiffness and angle of internal friction can be produced by adjusting the micro parameter $fric$ to obtain the desired value of internal friction and the micro shear stiffness $G_m$ to obtain a certain elastic stiffness. The influence of the micro poisson’s ratio $\nu_m$ is hardly visible.

- To obtain a certain poisson’s ratio and angle of dilatancy on a macroscopic scale seems not possible because both parameters are obtained as results and no steering is possible trough any input parameter. Especially the angle of dilatancy is linked to the angle of internal friction in a strong way. Increasing the internal friction gives an increasing angle of dilatancy. However such results have not been observed for the poisson’s ratio which remained almost constant during variation of each of the three micro parameters.

- The behaviour of the Swedish ‘Baskarp’ sand was successfully modelled by adjusting the micro parameters according to the described method. The found value for the micro shear modulus $G_m$ is similar to the measured value for quartz. Macroscopic quantities resulting from the biaxial test simulations were in accordance with those resulting from performed triaxial tests on the sand. The material behaviour as seen from the stress-strain curves resulting from the simulation was also similar to that of the triaxial tests.

- The ‘Baskarp’ sand could also be successfully modelled with the linear contact model.

- The ratio of maximum to minimum particle radius hardly influences the biaxial test simulation results until this ratio comes close to one and all the generated particles have nearly the same radius. When this is the case the particles tend to form a closed hexagonal packing which has a behaviour that deviates much from samples with larger ratio’s and a more varied particle radius distribution.

- At higher confining stresses, use of the Hertz-Mindlin contact model gives a realistic increase of sample stiffness, while the linear contact model shows hardly an increase of stiffness with increasing confining stress. Therefore when a wide stress range is needed in simulations, the Hertz model is preferred. For individual simulations at a certain stress, the linear contact model can be used by choosing the contact stiffness according to the expected sample stiffness for that stress state.
[Baars 1996]
Delft, 1996
APPENDIX VIII

GeoDelft report ‘Fluid flow in PFC2D’
Fluid flow in PFC2D

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January 2002
N:\projecten.afd\386730 - Hydraulic

The survey was performed for:
DELFRA C CONSORTIUM
DELFT

DEPARTMENT STRATEGIC RESEARCH
Project manager : ir. A. Bezuijen
Project supervisor : dr.ir. P. van den Berg

GeoDelft
Stieltjesweg 2, 2628 CK DELFT
Postbus 69, 2600 AB DELFT
The Netherlands

Telephone (+31) 15 - 269 35 00
Telefax (+31) 15 - 261 08 21
Postal account 234342
Bank MeesPierson NV
Account 25.92.35.911
The distinct element code PFC2D is being used for hydraulic fracturing calculations and has been extended with fluid flow. In this report, the implementation of fluid flow in the distinct element code PFC2D is presented and verified. The fluid flow agrees well with known Darcy flow and one-dimensional consolidation.

Also the interaction of pore fluid with particles of the distinct element method is described. Two types of interaction are discussed. A one-way interaction where pore pressures give rise to external force on the particles but particle movement doesn’t change the pore pressures and a fully coupled interaction of particles with pore-fluid where particle movement also changes the pore pressures which in turn affect the particle movement. Both the implementation as well as practical aspects of computation time are discussed.

Results show that fluid flow with one-way interaction of pore-fluid with particles has been successfully implemented and also can be used with comparative ease in PFC2D. The fully coupled interaction however suffers from being computationally very expensive although results from one-dimensional undrained compression and consolidation simulations agree well with theory.

It is recommended to use the one-way coupled interaction for the hydraulic fracturing simulations. If injection controlled calculations are preferred, the borehole can be modelled fully coupled while the rest of the sample uses one-way interaction. This leads to a calculation that is not much more expensive computationally.
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1 Introduction

In this report, the implementation of fluid flow in the two-dimensional discrete element code PFC2D is described and tested. The goal is to be able to prescribe certain fluid pressures and make time dependent flow calculations in combination with the movement of the discrete element particles for the application of hydraulic fracturing. At present the fluid and particles interact in such a way that the fluid pressures give rise to extra forces on the particles. The particle movement takes place under these external forces. Also, the change in fluid pressure due to the movement of the particles has currently been implemented, resulting in fully coupled flow-particle behaviour. But this is very time consuming. Usually only a one-way interaction is used where particle movements don’t give rise to extra pressure. For the case of hydraulic fracturing, the borehole can be fully coupled while the other parts of the model remain “one-way coupled” with no change in fluid pressures due to particle movement.

First, in Chapter 2, the implementation of fluid flow is described and the theory is developed. Chapter 3 describes several one-dimensional fluid flow calculations that were made and the results are compared with analytical solutions. This leads to a relationship between the permeability and compressibility constants on a micro level and those on macroscopic scale. In Chapter 4, a description is given of a simple two-phase flow model that has been implemented in the code. Calculations have been made for the one-dimensional flow situation to see if the results are in accordance with expectations. This two-phase flow could be useful for the hydraulic fracturing problem where for example a viscous oil is injected in the borehole while the surrounding soil is initially fully saturated with water. Chapter 5 describes the interaction of fluid with the particles.
2 Theory

In this chapter, first the implementation of fluid flow in the two-dimensional discrete element code PFC2D is described. Then, the theory is developed for one-dimensional fluid flow. This theoretical investigation leads to a relation between the micro flow parameters and those on macroscopic scale. In the next chapter these relations will be verified by comparing calculations with the analytical results.

2.1 computational aspects

For the fluid flow calculation, some sort of ‘mesh’ has to be created that is suitable for fluid flow. This mesh exists in the form of closed rings of particles that are in contact with each other and are found in the discrete element assembly, see Figure 2.1.

![Figure 2.1: domain structure used for fluid flow in PFC2D.](image)

Such a closed ring of particles is called a domain. It is assumed that over such a domain the fluid pressure is constant. Of course, in the distinct element code PFC2D, the particles move and contacts are sometimes deleted and sometimes created. Therefore the implemented domain routine updates the domains if this is the case. When a contact is deleted, usually two domains merge and when a contact is created, usually a domain splits. The domain structure is constantly being updated so it can be used for fluid flow. In the code, fluid flow is made possible through the contacts of the domains. For each contact it is known which two domains belong to it. The assumption is made that a contact acts as some sort of pipe through which flow occurs and the flow rate is directly proportional to the pressure difference:

\[ q_c = C_1(p_{dom1} - p_{dom2}) \]  

(2.1)
Here $q_c$ is the flow rate through a contact and has the dimension of $[m^2/s]$ because of the two dimensional geometry. $p\text{\_dom1}$ and $p\text{\_dom2}$ are the pressures in domain one and two of the contact and $C_1$ is a proportionality constant which is to be determined later. The flow calculation progresses in time with steps $\Delta t$. At a given time, the pressures in the domains have a certain value and all the flow rates $q_c$ for each contact are known. Then the total volume flow $\Delta V$ into a domain can be calculated for that time step by summing $q_c \Delta t$ for each contact of the domain. This gives rise to a pressure change because the fluid has a certain compressibility:

$$\Delta p = C_2 \frac{\Delta V}{V\text{\_dom}}$$

(2.2)

Where $V\text{\_dom}$ is the pore volume or in this case (pore) area of the domain. Accordingly, the pressure change in the domains can be calculated and a new pressure field is created that is used for the next step of the calculation.

The quantities $C_1$ and $C_2$ have to be determined from analytical solutions for groundwater fluid flow.

### 2.2 One-dimensional fluid flow

To determine the constants for the calculation, a one-dimensional fluid flow problem is considered. The geometry used for the one-dimensional flow is displayed in Figure 2.2. The total area has a width $W$ and a height $H$. On the left and right are two equal sized areas in which a prescribed high pressure $p_h$ and a low pressure $p_l$ are present as boundary conditions. The centre area has a length $L$. At the start of the calculation, the pressure in the centre area is set to $p_l$. If the whole sample would be a homogeneous material then, as time progresses, the pressure in the centre area would in the end be a linear decrease from $p_h$ at the left boundary to $p_l$ at the right boundary, according to the solution of the steady state potential flow problem. With a pressure gradient of $(p_h - p_l)/L$.

![Figure 2.2 Geometry for the one-dimensional flow calculation](image-url)

According to Darcy’s law, the flow rate in the $x$ direction then becomes:
Here, $\kappa$ is the intrinsic permeability constant and $\mu$ the dynamic viscosity of the fluid. The total flow rate is $Q = Hq_x$. This can be compared with the results from the calculation. Because the top and the bottom walls are closed, there is no flow in the $y$ direction.

A homogeneous material was modelled in the discrete element code PFC2D using a constant particle radius of 0.2 m, and a regular-packed assembly of the particles. Two types of packing were chosen. The first is the hexagonal closest packing, see Figure 2.3 and the second is a ‘square’-packed assembly as shown in Figure 2.4. These two types of packing are two extremes of a material with minimum and maximum porosity. The area is taken 18x8 meters for the square packed assembly, so there are 45x20 particles. For the hexagonal packed assembly the area is taken 18.2x8.2 meters and there are 45x23 particles. The white coloured line of particles in the middle is formed of connected balls from the bottom to the top closest to the line $x=0$ which is the symmetry line of the sample. These particles have to be known because it’s necessary to know all the contacts in a cross section for the calculation of the total flow rate $Q$, which is the sum over the flow rates through the contacts between the white coloured particles in the middle. On the left there is a light coloured area of particles which is the area with the prescribed pressure $p_h$.

For comparison with the regular packed assemblies, also a non-regular random sample was created using the same method as described in the report “Biaxial test simulations in PFC2D” [GeoDelft 1999]. Here, a minimum radius of 0.15 m and a maximum radius of 0.2 m were used for generation of the sample, with a porosity of 0.17. The result is shown in Figure 2.5. Because of the random packing, the sample should also be homogeneous when seen from a macroscopic perspective and calculations should give similar results.
Figure 2.3 The regular hexagonal closest packing assembly

Figure 2.4 The regular square packed assembly.
Using the initial pressures as described earlier and while performing the calculation, the pressure will eventually arrive at a steady value in all the domains, because the prescribed boundary conditions remain fixed in time. Then the flow through each contact remains constant also and the inflow in a certain domain is equal to the outflow. Because of the homogeneous material, the final result of the calculation will also be a linear decreasing pressure having globally the same pressure gradient. With this, the total flow rate $Q$ in the steady state situation can be calculated for the two regular structures.

First, this is done for the closed hexagonal packing, see Figure 2.6:
Shown are the equal-sided triangles that form the domains of which the centre is displayed with a dot. For the discussed flow problem, the domain centres that are at the same horizontal position (that are exactly above each other) have the same pressure at the beginning of the calculation. Because of symmetry, this will be true for the entire calculation. The horizontal distance between the domain centres is equal to the radius $r$, as shown in Figure 2.6. Then, the pressure gradient can be approximated by:

$$\frac{\partial p}{\partial x} \approx \frac{p_{\text{dom}i+1} - p_{\text{dom}i}}{r} \quad (2.4)$$

The implemented flow rate $q_c$ through contact $c$, see Figure 2.6, is according to (2.1):

$$q_c = C_1 (p_{\text{dom}i} - p_{\text{dom}i+1}) = -rC_1 \frac{\partial p}{\partial x} \quad (2.5)$$

The flow rate $q_c$ through all the contacts at the same horizontal position has the same value. To obtain the total flow rate $Q$ through the cross section, the number of contacts in the line of particles from bottom to top (see Figure 2.3) has to be calculated. From Figure 2.6 it can be seen that one contact has a vertical distance of $r\sqrt{3}$. In the problem the height $H$ of the sample is chosen in such a way that an integer number of particles fit precisely. The top and bottom particles have no contact anymore, so the exact number of contacts $n_c$ becomes:

$$n_c = \frac{H - 2r}{r\sqrt{3}} \quad (2.6)$$

For a particle radius much smaller than $H$, the term $2r$ can be neglected. Then the total flow rate $Q$ becomes:

$$Q = n_c q_c = -\frac{H}{r\sqrt{3}} rC_1 \frac{\partial p}{\partial x} \quad (2.7)$$

Compared with the analytical value $Q=Hq_x$, with $q_x$ as in (2.3) the constant $C_1$ can be calculated:

$$C_1 = \sqrt{3} \frac{\kappa}{\mu} \quad (2.8)$$

For which it is expected that equation (2.1) will give exact results for the hexagonal packing.

Now, the square packed case is considered, see Figure 2.7:
The horizontal distance between the domain centres is now $2r$ and pressure gradient becomes:

$$\frac{\partial p}{\partial x} = \frac{p_{dom_{i+1}} - p_{dom_i}}{2r}$$  \hspace{1cm} (2.9)$$

And the flow rate through contact $c$:

$$q_c = C_1(p_{dom_{i}} - p_{dom_{i+1}}) = -2rC_1 \frac{\partial p}{\partial x}$$  \hspace{1cm} (2.10)$$

Now, the number of contacts in the cross section is:

$$n_c = \frac{H - 2r}{2r}$$  \hspace{1cm} (2.11)$$

Again, the term $2r$ in the numerator can be neglected when the particle radius is small compared to the model geometry. For this geometry, the total flow rate is:

$$Q = -HC_1 \frac{\partial p}{\partial x}$$  \hspace{1cm} (2.12)$$

And when again comparing to Darcy’s law, $C_i$ becomes:

$$C_i = \frac{\kappa}{\mu}$$  \hspace{1cm} (2.13)$$

The hexagonal closest packing and the square packing represent two extremes in geometry. The difference between them is a factor of $\sqrt{3}$ in the first implemented equation (2.1).
2.3 One-dimensional consolidation

By looking at Darcy flow, the constant $C_1$ in the implemented PFC fluid flow equation (2.1) has been found exactly for square and hexagonal packings. To find the constant $C_2$ defined in equation (2.2), we look into one-dimensional consolidation. First, the general equations and analytical solution will be discussed and after that the equations will be used to find the constant $C_2$.

2.3.1 Equations and analytical solution

The equation for one-dimensional consolidation is given by (see for example [Verruijt 1993]):

$$\frac{\partial \varepsilon_{xx}}{\partial t} = -n\beta \frac{\partial p}{\partial t} + \kappa \frac{\partial^2 p}{\partial x^2}$$

(2.14)

Where $\beta$ is the compressibility of the fluid, $n$ is the porosity and $\varepsilon_{xx}$ is the strain in the direction considered, in this case the $x$-direction. The one-dimensional stress strain relationship using linear elasticity is given by:

$$\sigma' = -(K + \frac{4}{3}G)\varepsilon_{xx}$$

(2.15)

Where $\sigma'$ is the effective stress in $x$-direction, $K$ the bulk modulus and $G$ the shear modulus of the medium. This relation is more conveniently written:

$$\varepsilon_{xx} = -m_v\sigma'$$

(2.16)

Substituting equation (2.16) in (2.14) using Terzaghi’s principle $\sigma' = \sigma - p$, where $\sigma$ is the total stress in $x$-direction and $p$ the fluid pressure, gives:

$$(m_v + n\beta) \frac{\partial p}{\partial t} = \kappa \frac{\partial^2 p}{\partial x^2} + m_v \frac{\partial \sigma}{\partial p}$$

(2.17)

Which is the general one-dimensional consolidation equation for a linear elastic medium with Darcy flow. A special case is when during consolidation the total stress $\sigma$ remains constant. Then, equation (2.17) can be written as:

$$\frac{\partial p}{\partial t} = c_v \frac{\partial^2 p}{\partial x^2}$$

(2.18)

$$c_v = \frac{\kappa}{\mu (m_v + n\beta)}$$

Where $c_v$ is called the consolidation coefficient. We write the analytical solution for a sample of length $L$, such as shown earlier in Figure 2.2. Let the initial condition at $t=0$ be $p=p_0$ over the length of the sample. Then, as boundary conditions at the left and right boundaries we set $p=0$ (equivalent to
$p_n=0$ and $p_l=0$ in Figure 2.2). This problem can be solved analytically [Verruijt 1993]. When the boundaries are chosen at $x=0$ and $x=L$, the analytical solution is given by:

$$
\frac{p(x,t)}{p_0} = \sum_{j=1}^{\infty} \frac{(-1)^{j-1}}{2j-1} \cos \left( (2j-1) \frac{\pi}{L} (1 - \frac{x}{L}) \right) \exp \left( -(2j-1)^2 \frac{\pi^2 c_i^2 t}{L^2} \right)
$$

(2.19)

### 2.3.2 Consolidation in PFC2D

For the moment we only look at fluid flow in PFC2D without deformation of the skeleton, or in the PFC2D case, no particle movement. Then, the consolidation is a pure diffusion process. In Chapter 5, consolidation with deformation will be discussed. The equation for no deformation can be found by letting the stiffness of the skeleton go to infinity, hence $m_v=0$ in (2.18). The form of the equation (2.18) doesn’t change then, only the consolidation coefficient is now given by:

$$
c_v = \frac{\kappa}{\mu n \beta}
$$

(2.20)

The equation for zero deformation during consolidation can also directly be found from (2.14) by setting:

$$
\frac{\partial \varepsilon}{\partial t} = 0
$$

(2.21)

Which means a strain rate of zero during the consolidation process.

For the case with zero deformation given by equation (2.18) using the consolidation coefficient from (2.20), the constant $C_2$ in equation (2.2) can be determined by comparing the implemented flow equations with a discrete formulation of equation (2.18), just as $C_1$ was determined using a discrete formulation of Darcy flow. The analytical solution will be used in the next Chapter to verify the implemented fluid flow equations with the derived constant $C_2$. If a finite difference method is applied to the equation (2.18) with distance of $\Delta x$ between the points and time step $\Delta t$, the discrete formulation of (2.18) for zero deformation is given by:

$$
\frac{\Delta p(x)}{\Delta t} = \frac{\kappa}{\mu n \beta} \frac{p(t, x - \Delta x) - 2p(t, x) + p(t, x + \Delta x)}{(\Delta x)^2}
$$

(2.22)

Here $\Delta p(x)$ is $p(t+\Delta t, x) - p(t, x)$, also the increase in time of the pressure at position $x$.

In case of the flow implementation in PFC2D, the quantity $\Delta V$ in equation (2.2) is the difference between inflow and outflow of domain $i$. For the one-dimensional flow situation in case of the square or hexagonal regular packed assemblies this becomes:

$$
\Delta V = (q^{i-1}_c - q^i_c) \Delta t = C_1 (p_{i-1} - 2p_i + p_{i+1}) \Delta t
$$

(2.23)
Here, $q_{ci}^{i-1}$ is the flow rate from domain $i-1$ to domain $i$ and $q_{ci}^i$ is the flow rate from domain $i$ to domain $i+1$. With (2.23), equation (2.2) becomes:

$$\Delta p = \frac{C_1 C_2}{V_{domi}} (p_{i-1} - 2p_i + p_{i+1}) \Delta t$$

(2.24)

For the hexagonal closest packing the (pore) area of the domains is $r^2(\sqrt{3} - \pi/2)$, whereas $C_1 = \sqrt{3} \kappa/\mu$ and the horizontal distance between domain centres $\Delta x = r$. With this, (2.24) can be rewritten:

$$\frac{\Delta p}{\Delta t} = \frac{\sqrt{3}}{\sqrt{3} - \frac{\pi}{2}} \frac{\kappa C_2}{\mu} \frac{(p_{i-1} - 2p_i + p_{i+1})}{r^2}$$

(2.25)

Comparing this with the discrete equation for one-dimensional consolidation (2.22) leads to the conclusion that for the hexagonal closest packing:

$$C_2 = \frac{\sqrt{3} - \frac{\pi}{2}}{\sqrt{3}} \frac{1}{n\beta}$$

(2.26)

For the square packed situation, the domain volume is $(4-\pi)r^2$, constant $C_1 = \kappa/\mu$ and $\Delta x = 2r$. This gives:

$$C_2 = \frac{4 - \pi}{4} \frac{1}{n\beta}$$

(2.27)

Given that the porosity for the hexagonal closed packing case is $n = (\sqrt{3} - \pi/2)/\sqrt{3}$ and for the square packed case $n = (4-\pi)/4$, the constant $C_2$ for both cases is the same, namely:

$$C_2 = \frac{1}{\beta}$$

(2.28)

Which is logical, since $C_2$ is the bulk modulus of the fluid and $\Delta V/V_{dom}$ in equation (2.2) is the volumetric strain. With the implementation of equation (2.2) in the PFC2D code, however, one needs to be careful. This is because the code is two-dimensional and caution must be taken in the calculation of the domain volume $V_{dom}$. Just now we calculated it for the hexagonal case by calculating the area of triangular shaped domain $r^2\sqrt{3}$ and subtracting that area of the three particles that lies within the triangle $3*1/6*\pi r^2$, resulting in a domain volume $V_{dom} = r^2(\sqrt{3} - \pi/2)$ per meter in the 3rd dimension. In this view, the particles were taken as long cylinders to calculate the domain volume. The resulting porosity is then $(\sqrt{3} - \pi/2)/\sqrt{3} = 0.0931$ for this “cylinder view”. Whereas the porosity of the closest packing of actual balls in 3D with radius $r$ is 0.2595 (from the PFC2D manual) and larger than for the cylinder view. This means that compared to a real-life material, the porosity calculated from a “cylinder view” is more than a factor of 2 too low giving domain volumes that are too low and a fluid behaviour that is too stiff because the quantity $C_2\Delta V/V_{dom}$ being too high for a given inflow $\Delta V$. 

12
What’s wished for in the PFC2D code is flow behaviour that is realistic in the sense that it can be compared to real materials and not cylinder like materials. Therefore it’s necessary to look for a way around this problem of calculating the porosity and with it the domain volume $V_{dom}$. This is discussed in the next section.

### 2.4 Porosity

In the previous section it has been shown that there are considerable differences in porosity between similar particle packings in the two- and three-dimensional situations. These differences can lead to over a factor two error in the calculation of the domain volume (the pore volume).

In the discrete element simulation there is another problem. Particles have what can be called “soft contacts”. Namely, when pressures are applied on a material that’s modelled with particles, the particles will overlap and the contact force is a function of the distance that the particles overlap, linear or non-linear. For very stiff materials, the overlap is small because the contact stiffness is very high. But for softer materials it is possible that, for a randomly generated sample, the particles will overlap so much that they will leave no pore volume in a domain when the domain volume is calculated according to the 2D “cylinder view”. For those domains this would lead to a negative pore volume in the calculations causing great instabilities in the code. It is then important to look for other ways of calculating the porosity and pore volumes of the domains to find a way to prevent this from happening and also to obtain a realistic value for the porosity.

The definition of the porosity $n$ for actual 3D materials is:

$$n = \frac{\text{total volume} - \text{volume of soil particles in total volume}}{\text{total volume}}$$

(2.29)

The porosity calculated according to the 2D “cylinder view”, as discussed before in the previous section we define here as being the two-dimensional porosity $n_{2D}$:

$$n_{2D} = \frac{\text{area of domain} - \text{area of circles in the domain}}{\text{area of domain}}$$

(2.30)

Here, the area of the domain is the area of the polygon formed by connecting the centres of the particles (2D circles) making up the domain. And the area of circles inside the domain is the area of the part of the particles that lies inside that polygon.

We can also try to calculate a kind of quasi three-dimensional porosity from the two-dimensional particle assembly in PFC2D. The idea is to calculate the volume of a ball instead of a cylinder and divide that by $2r$ where $r$ is the particle radius. In this way the area of the particles is effectively less. The “cylinder view” gives for a particle area the area of a circle with radius $r$, namely $\pi r^2$. In the “ball” situation, the volume of a ball with radius $r$ is $\frac{4}{3}\pi r^3$. This divided by the height of the ball $2r$ gives as effective area: $2\pi r^2/3$, which is a factor $2/3$ times the normal area. With this, we can make a second definition of porosity, which we call the quasi three-dimensional porosity $n'$:
\[
\frac{\text{area of domain} - \frac{2}{3} \text{area of circles in the domain}}{\text{area of domain}} = n'
\]

(2.31)

Which is similar to the definition of \( n_{2D} \) only the area of particles inside the domains is diminished with a factor 2/3:

These two porosity’s \( n_{2D} \) and \( n' \) can be expressed in each other with the relations:

\[
\begin{align*}
n' &= \frac{1}{3} + \frac{2}{3} n_{2D} \\
n_{2D} &= \frac{3}{2} n' - \frac{1}{2}
\end{align*}
\]

(2.32)

To compare these three porosity definitions, again the closest hexagonal packing and square or cubic packing are considered, see Table 2.1. Now it can be seen that for the square or cubic packing the quasi 3D porosity \( n' \) is the same as the three-dimensional porosity \( n \). For the hexagonal situation, the porosity \( n' \) is much larger that that of the three-dimensional porosity, which was expected. So for closely packed assemblies, the quasi three-dimensional calculation of the porosity leads to values that are too large.

<table>
<thead>
<tr>
<th>Packing</th>
<th>( n_{2D} )</th>
<th>( n'(\text{quasi 3D}) )</th>
<th>( n (3D) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>closest packing</td>
<td>0.0931</td>
<td>0.3954</td>
<td>0.2595</td>
</tr>
<tr>
<td>square packing</td>
<td>0.2146</td>
<td>0.4760</td>
<td>0.4760</td>
</tr>
</tbody>
</table>

Table 2.1 Comparison of different definitions of porosity in 2D, quasi 3D and 3D.

An advantage of using the quasi three-dimensional approach in calculating the domain pore volumes and the porosity is that it is very unlikely to find domains with a negative pore volume and porosity. Only when a very soft stiffness is chosen for the particles, can such a phenomenon occur. In the modelling of soils, such a thing will not happen.

Although a two-dimensional discrete element code is used, it's useful to try to simulate the behaviour as it would be in three dimensions. In a real material the local porosity may change because of it’s irregular packing, but in measurements a global porosity is measured. In the PFC2D model, the porosity in the domains also varies. However, the code uses the porosity \( n_{2D} \) to generate the assembly.

Through linear interpolation, the porosity \( n \) can be connected to \( n' \):

\[
n' = 0.476 - \frac{0.476 - n}{0.476 - 0.2595} (0.476 - 0.3954)
\]

(2.33)

It can be seen from (2.33) that when \( n=0.476 \), the porosity for the cubic packing, the porosity \( n' \) also is 0.476 which is correct according to Table 2.1. When \( n=0.2595 \), the porosity for the hexagonal packing, \( n'=0.3954 \), which is also correct according to Table 2.1. So the user could give the three-dimensional porosity and with (2.33) a good guess can be made of the quasi three-dimensional
porosity. With equation (2.32), the two-dimensional porosity can then be calculated. This $n_{2D}$ is then used to create the particle assembly.

After the particle assembly has been generated and during the flow calculation, the program calculated the quasi three-dimensional porosity. From this with the reverse of equation (2.33), the three-dimensional porosity $n$ can be calculated for each domain and used in the calculation. In this way it’s likely that the sample has a realistic average porosity which should be close to the porosity given by the user and at the same time porosity variations exist in the sample.

### 2.4.1 Porosity used in current PFC2D code

The quasi 3D porosity $n'$ has been implemented and turned out to be stable in the sense that no negative domain volumes appeared during calculations for realistic soil stiffness parameters. However, it turned out to be very difficult for the user to have good control over the porosity if it’s being calculated with a quasi 3D case, even when using interpolation discussed in the previous section. For this reason a different method is adapted for the moment. Namely the user can give a value for the porosity wished for and the code calculates the pore volumes of the domains by multiplying this user given porosity with the area of the domain. This eliminates instabilities and gives control over the porosity to the user.

When this approach is used in hydraulic fracturing simulations, the borehole is treated differently from the other domains. The domain volume of the borehole is calculated then according to the cylinder view, namely the area of the borehole polygon minus the area of the part of the particles inside the borehole domain. Porosity is of course nearly one for larger boreholes. If the volume would be calculated according to the user porosity, it would be far off.

For more sophisticated problems where permeability depends on the porosity, the quasi 3D porosity $n'$ would still be of some value. For the remainder of this report it is not used to verify the implementation of the flow equations (2.1) and (2.2) in PFC2D.
3 Calculations

In this chapter, several calculations are made to test the theory discussed in the previous chapter and to gain more insight into flow calculations within the two dimensional discrete element code.

3.1 Verification of the total flow rate Q

For the one-dimensional problem discussed in the previous chapter, calculations are made with the hexagonal closest packed, square packed and random assemblies, see Figure 2.3, Figure 2.4 and Figure 2.5. As boundary conditions, the pressure in the left area, see Figure 2.2, has been chosen \( p_h = 1.6 \text{ MPa} \) and the pressure \( p_l \) in the right area has been set to zero. As initial condition, the pressure in the centre area is set to zero as well.

First it is verified for the hexagonal packing that with time progressing, the pressure approaches the linear decreasing function with \( x \), and a constant pressure gradient over the sample. This pressure function is determined by defining a horizontal line at \( y=0 \), the middle of the sample (in the program the sample has dimensions \(-0.5H \) to \( 0.5H \) in \( y \) and \(-0.5W \) to \( 0.5W \) in \( x \)). The pressures of the domains with their domain centre closer than half a particle radius to that line are written to a file together with their \( x \)-positions during the calculation. This allows for monitoring the pressure as function of \( x \). As mentioned earlier, the modelled area \( H \times W = 8 \text{ m} \times 18 \text{ m} \). The left and right areas where the boundary pressures are prescribed are taken to be \( 3 \text{ m} \) in width, so then \( L = 12 \text{ m} \). The constant \( C_1 \) in equation \( (2.1) \) is set to \( \sqrt{3\kappa/\mu} \), so exact results are to be expected for the hexagonal packing. The value of the constant \( \kappa/\mu = 1.0 \times 10^{-8} \text{ m}^2/\text{sPa} \). The constant \( C_2 \) was taken \( 1/\beta \) and the pore volumes of the domains were calculated according to the method described in the previous chapter, multiplying the polygon volume with a user defined porosity. The value of \( C_2 \) is not relevant for determining the flow rate in a steady state situation, so the quantity \( n\beta \) is set to 1, choosing \( n = 0.4 \) and \( \beta = 1/0.4 \). The result for a calculation with 30000 time steps is shown in Figure 3.1:

![Figure 3.1 Pressure function for progressing time](image-url)
Initially, at time step \( t=0 \), the pressure function is the step function of 1.6MPa over the left area until \( x=-6m \), and zero for larger \( x \). As time progresses, the function is almost linear at time step \( t=30000 \). This shows that the pressure gradient is indeed constant over the length \( L \) after a certain time, when the steady state flow situation is reached. For the case of the square packed and random assemblies, similar results were observed all giving an almost constant pressure gradient after a large number of time steps.

During the calculation, the total flow rate as a function of time can be calculated according to the method described in the previous chapter. Namely, the total flow rate \( Q \) is the sum over the flow rates \( q_c \) through contacts of connecting particles forming a line from the bottom to the top of the sample, which is located in the centre of the sample, see Figure 2.3, Figure 2.4 and Figure 2.5. This is done with parameters as given previously for the hexagonal packing with the constant \( C_1 \) in equation (2.1) still \( \sqrt{3} \kappa/\mu \). Also \( n_\beta \) is the same and equal to unity. The results are shown in Figure 3.2:

![Graph showing total flow rate as a function of time for hexagonal, square packed and random packed assembly.]

Figure 3.2 The total flow rate as a function of time for the hexagonal, square packed and a random packed assembly.

It can be seen that in the steady state situation, the flow rate for the hexagonal case is \( 1.0E-2 \text{ m}^2/\text{s} \). Analytically \( Q=H\kappa/\mu (dp/dx) \) which gives for this case \( Q=1.06e-2 \text{ m}^2/\text{s} \), which agrees well with the calculation result for the hexagonal packing. The flow rate in the steady state situation for the square packed assembly is \( 1.7E-2 \text{ m}^2/\text{s} \), which is indeed a factor \( \sqrt{3} \) larger than the flow rate for the hexagonal case. This was expected, because the constant \( C_1 \) was chosen as \( \sqrt{3} \kappa/\mu \) and according to the theory of the previous chapter, the square packed assembly would yield exact results if \( C_1=\kappa/\mu \). The flow rate for the random assembly is \( 1.17E-2 \text{ m}^2/\text{s} \), which is between the two extremes of hexagonal and square packed assemblies. Such a random packed assembly consists mostly of triangular shaped domains, with some larger domains with four or more particles. Therefore, flow characteristics closer to those of the hexagonal packing were expected and were also found, see Figure 3.2.

The result is that the permeability is effectively larger for a more porous structure, which is also realistic. However, this is very different from the dependence of the permeability on the porosity that can be found in the literature. Here the difference in permeability is at most a factor \( \sqrt{3} \).
Figure 3.2 also shows a similar time dependent behaviour of the two situations, however, the steady state is reached a little sooner for the square packed assembly. This is due to the consolidation coefficient depending on both the permeability and compressibility. The compressibility characteristics are the same for the three cases with \( n\beta =1 \), but because \( C_f \) was chosen to give exact results for the hexagonal packing, the permeability for the square packing is larger than for the hexagonal packing, resulting in a larger consolidation coefficient. This time-dependent behaviour will be further investigated in the next section when consolidation is discussed.

3.2 Verification of one-dimensional consolidation without deformation

For one-dimensional consolidation, the problem discussed in section 2.3 is simulated in PFC2D, without deformation of the particles. Now the prescribed boundary pressures are \( p_h = p_l = 0 \) and as initial condition, the pressure in the centre area has been set to 1.6 MPa. During the calculation, the pressure will decrease in the sample and become zero after a long period, which is the steady state solution of the problem. The permeability is taken \( \kappa/\mu = 1.0 \times 10^{-8} \text{ m}^2/\text{sPa} \), the compressibility \( \beta = 1.0 \times 10^{-7} \text{ Pa}^{-1} \) and for the porosity \( n = 0.4 \) was taken. The consolidation calculation is made for the hexagonal closest packing, so the constants used in the calculation were calculated from equations (2.8) and (2.26) giving \( C_f = 1.73 \times 10^{-8} \text{ m}^2/\text{sPa} \) and \( C_s = 1/\beta \), when domain volumes are calculated as described earlier by multiplying the polygon area with the porosity \( n = 0.4 \). The calculation is verified with the analytical solution of the problem given in (2.19), using the consolidation coefficient \( c_v = \kappa/(\mu n \beta) = 0.25 \text{ m}^2/\text{s} \). The results are shown in Figure 3.3:

![Figure 3.3 Comparison of the numerical (PFC2D) and analytical solution of the one-dimensional consolidation problem for the hexagonal packed assembly. The time \( t \) is measured in the number of time steps. The time in the analytical formula is the time step size for fluid flow used in PFC multiplied with the number of time steps.](image)

The numerical solution agrees very well with the analytical results, as was to be expected after deriving the equations in the previous chapter. However, here the porosity was given by the user and exact. Results are expected to differ from the analytical results if domain volumes are calculated with some other porosity definition like the quasi 3D case for example.
Now, a calculation is made with the random packed assembly as was shown earlier in Figure 2.5. The permeability for this particle assembly was 1.17 times higher than that for the hexagonal structure as was seen earlier. In order to obtain a permeability of $k/\mu = 1.0 \times 10^{-8}$ m$^2$/sPa as used in the analytical consolidation calculation, now the permeability used for the flow calculation has to be divided by 1.17 giving the input parameter, $k/\mu = 0.855 \times 10^{-8}$ m$^2$/sPa. The compressibility and porosity remain unchanged with $\beta = 1.0 \times 10^{-7}$ Pa$^{-1}$ and $n=0.4$. The consolidation coefficient used in the analytical solution remains the same also, $c_v=0.25$ m$^2$/s and with it the analytical solution.

The result of the one-dimensional consolidation simulation using these parameters is shown in Figure 3.4:

![Figure 3.4 Result of one-dimensional consolidation for the random assembly compared with analytical solution.](image)

The non-regular discretisation is clearly visible. And the results agree well with the analytical solution.
4 Two-phase flow

In the previous chapters, the implementation of fluid flow in the discrete element code PFC2D has been described and tested. The results were found to be in accordance with known analytical results. In this chapter, a simple two-phase flow model that also has been implemented in the code is described and tested. Two-phase flow is important for the hydraulic fracturing problem, because oil is injected in the borehole while the surrounding soil could for example be fully saturated with water. Oil is more viscous and causes a lower permeability. This leads to a pressure gradient that is steeper close to the borehole and less steep in the area containing only water. This difference in pressure distribution compared to single phase flow could lead to a different fracturing behaviour.

4.1 Implementation issues

As described earlier, the flow calculation describes flow through contacts of the domains. In the two-phase flow, two fluids are present, phase one (fluid one) and phase two (fluid two). To describe the two-phase flow, a degree of saturation $S$ has been defined for each domain. The value of $S$ is between zero and one. If $S=0$ then only phase one (fluid one) is present in that domain. If $S=1$, the domain contains only phase two (fluid two).

The basic assumption that has been made for the two-phase flow implementation is that a certain domain will not produce phase two unless it is fully saturated with phase two and if fully saturated with phase two, the domain will only produce phase two. This means that if the pressure is such that through a contact something flows out of the domain, only phase one will flow out of the domain until that domain has a saturation $S=1$. Then only phase two can flow out of the domain until the saturation $S$ becomes smaller than one again. There is no such condition on the inflow, since the inflow is always an outflow from some other domain.

Because the fluids have a different viscosity’s $\mu_1$ and $\mu_2$, which results in a different $\kappa/\mu$ factor. The $\kappa/\mu_1$ factor of fluid one is used for the flow through a contact if fluid one flows through that contact and the $\kappa/\mu_2$ of fluid two is used when fluid two flows through the contact. In the program it is known which of the two domains for a contact has highest pressure, so the flow direction is known. If the domain with highest pressure has $S<1$, then fluid one flows through that contact and the corresponding permeability is chosen for that contact.

Also, currently it is assumed that the compressibility of the two fluids is equal, which is probably true for oil and water.

This model has been implemented in the existing code. The saturation $S$ is cut off should it go below zero or rise above one. Then, to prevent numerical problems, a domain is considered to be fully saturated with phase two if $S>0.9$. In this way a numerical unstable situation is prevented. Namely, if $S=1$ was used as condition, in one flow step $S$ could become equal to one. Then, in the next flow step the domain starts to produce phase two, and due to the numerical process and inaccuracies of mass balance this could cause $S$ to drop below one again making the domain produce phase one again. Such situations would make a domain produce phase two on and off. In the present situation where $S>0.9$ is used, while the cut off still lies with $S=1$, the saturation can be greater than 0.9 and should it drop
slightly in one step, the domain would still produce phase two. Only when after several steps it would really drop below 0.9 would fluid one be produced again.

Now other than the prescribed pressures as boundary conditions and initial pressures also the saturation has to be given. The program handles a given saturation as such that where the pressure is fixed (prescribed boundary pressure), the saturation also doesn’t change.

4.2 Simulations

First, the one-dimensional problem is considered for the regular hexagonal packed assembly. A calculation similar to that in section 3.1 is made with the left area having a prescribed high pressure of 1.6 MPa and the right area a prescribed pressure of zero. Initially the centre area has a pressure of zero too. Now, also the initial saturation has to be given. In the left area \( S = 1 \), so this is completely phase two which is the higher viscous fluid here. In the right area \( S = 0 \). These values for the saturation are fixed. In the centre area, the saturation is set to zero initially. The compressibility has been chosen the same as in the one-dimensional consolidation calculation. The permeability/viscosity factor of fluid one has been chosen \( \kappa/\mu = 1.0 \times 10^{-8} \text{ m}^2/\text{sPa} \) and that of fluid two a factor four lower, namely \( \kappa/\mu = 2.5 \times 10^{-9} \text{ m}^2/\text{sPa} \).

The expected result will be that the fluid with higher viscosity is injected from the left and slowly penetrates the sample. The pressure curve will be steeper in the area that is penetrated, because there is a lower permeability. The result of the calculation is shown in Figure 4.1:

![Figure 4.1 The results of the one-dimensional two-phase calculation.](image)

At the different times, the crossover from phase two to phase one is visible as a distinct bend in the pressure curve. It can be seen that when time progresses the bend moves to the right, indicating a further penetration of the phase two fluid in the sample. In the final step, the pressure curve is again linear. At this time the sample has been fully saturated with phase two and has a constant permeability.
5 Interaction of particles with pore fluid

In the previous chapters, the various aspects of the implementation of fluid flow in PFC2D were discussed and verified. In this chapter, the interaction of pore fluid with the particles in PFC2D is discussed. There exist two variants of interaction, one-way interaction and fully coupled flow-particle interaction. In the one-way interaction, the fluid pressures in the domains are used to calculate external forces on the particles, but movement of particles don’t give rise to an additional fluid pressure. In fully coupled flow, the changes in domain volume due to particle movement are also calculated and the pressures in the domains are updated giving new external forces on the particles in turn causing deformations until equilibrium is reached. In this chapter both aspects of coupling are discussed.

5.1 One way coupling

Now the fluid flow has been modelled, there must be an interaction with the particles in order to have an effect in the distinct element simulation. Suppose that a certain particle is part of four domains, as shown in Figure 2.2. Then, in each of the domains surrounding the particle is a fluid pressure. These different pressures act on the particle. In the code, the pressures are integrated over the part of the circle (boundary of the particle) lying in the specified domain. This integration gives a contribution to the total force on the particle. The integration in each domain surrounding the particle is carried out and summed to give the total force by the fluid on the particle $F_{\text{fluid}}$.

![Fluid interaction with particles.](image)

For each particle the total force due to fluid pressure is calculated and the X and Y components of the force are stored in the external force addresses for each particle in PFC2D. Now, the standard PFC2D code uses this external force, in addition to the inter-particle forces, for the computation of the displacements.

This one-way interaction is very straightforward and no special considerations for stability need to be taken. Usually it is sufficient to calculate the external forces after a flow step and with the external forces remaining constant, a number of deformation steps are performed in PFC2D until equilibrium. Then, another flow step is made resulting in new pore pressures and new values for the external forces on the particles.
5.2 Fully coupled flow-particle interaction

The full interaction of pore fluid with particles starts from the one-way interaction described in the previous section. But now for movement of the particles due to the external fluid force, new domain volumes must be calculated giving rise to new fluid pressures and a change of external forces on the particles.

The way the coupling between solid particles and fluid flow is implemented in the PFC2D code is similar to a staggered analysis method in a finite element code. Where a fluid flow step and a deformation step are calculated separately. A flow step is taken whereby the pressure change is applied in a deformation calculation, from the deformation calculation a new pressure distribution is obtained which is used in a new flow step. How the fully coupled calculation is currently implemented is presented in Figure 5.2.

Figure 5.2: Flow chart of coupled simulation process.

The flow steps are performed with step size \( dt_{\text{flow}} \). The step size should be chosen as such that the flow calculation itself is stable. So for stability, this step size can be the same as for the uncoupled flow simulations, since no deformation has an effect on the resulting pressure field during a flow step.

The new pressure calculated in the flow step is then applied to the particles as external force (as was shown in Figure 2.2) and now a number of deformation steps are done until balance is achieved. After
each deformation step, the new domain volumes (pore volumes) are calculated and, from the volume difference, new pore pressures are calculated. Then, these new pressures are applied to the particles for another deformation step until an equilibrium is reached. The currently used criterion for equilibrium is that the average unbalance force divided by the average contact force has to be lower than a user given value. How the new pore volumes are calculated and how the pressure depends on the change of pore volume is discussed in the next subsection.

Normally, the PFC2D program calculates a stable time step for deformation analysis. But because of the increased stiffness due to the pore fluid between the particles, this time step has to be recalculated to obtain a stable time step. Later it will be shown how an estimation of a stable time step can be found.

5.2.1 Pore volumes and pore pressure

During the deformation the pore volumes change and the pore pressures change accordingly. This is the core of the coupled fluid-solid calculations. Suppose that a sample is created with a certain particle distribution. This is the initial state. As mentioned in Chapter 2, the fluid flow is described by creating a domain structure of polygons made up from connecting particles. Each polygon has a pore pressure value. The area of each polygon can be calculated, giving a volume (per meter sample in 3rd dimension). To obtain the real pore volume, this polygon volume has to be multiplied by the porosity. The porosity depends on the fraction of solid in the polygon. This gives rise to two problems:

1. The PFC2D program is a two-dimensional computer code, and porosity in two dimensions deviates quite a lot from that in three dimensions when the particles have a similar packing (for example cubic versus square of tetrahedral versus triangular). This was shown in sections 2.3 and 2.4. So comparing the results with three-dimensional problems is impossible if the porosity is based on a two-dimensional concept.

2. As shown, calculation (2D) of the porosity by subtracting the area of the particles that lie in the polygon from the polygon area can give very low porosity values in a random packed sample of different particle sizes. These in turn give rise to very low pore volumes for some domains. The pore pressure increases much faster when the pore volume is small, and if some pores have a very low pore volume, these pores give instabilities in the pressure calculation. In this case the time step has to be chosen even smaller just because of these few pores.

The coupled flow calculations are thus even more sensitive in this respect than the ordinary flow simulations without deformation. Both of the above problems are avoided here by choosing a fixed porosity value for the domains, as was already done in the fluid flow calculations. The porosity value is chosen according to the information that the user has about the material in question. For sands a porosity of 0.4 is common. Of course, as mentioned earlier, in case of the borehole simulations the borehole will be treated differently from the rest of the domains. Because for the borehole domain, the porosity value is no longer valid. Only for the borehole will the porosity and (with it the pore volume) be calculated directly by subtracting the particle area from the polygon area. The deviation from the 3D situation is small for the borehole since there is relatively little particle volume inside the borehole domain. It is assumed that choosing a fixed value for the porosity has little effect on the actual physics of the problem. Note that it’s still possible to have the permeability vary as a function of a calculated porosity as long as the function varies within well defined limits so that a stable time step can be computed.
So with a fixed porosity defined by the user, the initial pore volumes can be calculated by multiplying the polygon volume by the porosity \( n \). But during deformation the porosity changes, so it’s not correct to calculate the pore volume at a later time by multiplying the pore volume with the initial porosity.

As example a one dimensional compression test is shown, see Figure 5.3.

![Diagram of one dimensional compression test](image)

Figure 5.3: Pore volume changes in the one-dimensional compression test.

Initially, the sample has a porosity \( n \) and a total volume of \( V_0 = BL_0 \). Therefore, the initial total pore volume is \( nV_0 \) and the initial total volume occupied by the solid particles is \( (1-n)V_0 \). After compression the sample has a total volume of \( V_1 = BL_1 \). A commonly made assumption in soil mechanics is that the soil particles itself are incompressible, which means that the total volume of soil particles inside the sample does not change. Because the total volume is equal to the total pore volume plus the total volume of particles, the total pore volume after compression becomes:

\[
V_{1\text{ pore}} = V_1 - (1-n)V_0
\]  

(5.1)

Normally a linear relation is assumed between the pressure increase and the volume change:

\[
\Delta p = -\frac{\Delta V_{\text{pore}}}{V_{\text{pore}}} K_w
\]  

(5.2)

Here \( K_w \) is the bulk modulus of the pore fluid (2.0E9 Pa for pure water) and \( \Delta V_{\text{pore}} \) the change in pore volume. \( V_{\text{pore}} \) is usually understood to be the initial pore volume but, because of the relative high stiffness of the pore fluid, the difference would be very small if the current pore volume were used. This is a second order effect. The change in pore volume can be found by subtracting the initial pore volume \( nV_0 \) from (5.1). This gives for the pressure change:

\[
\Delta p = -\frac{V_1 - V_0}{nV_0} K_w
\]  

(5.3)

The pore volume change, which is the numerator in (5.3), is equal to the difference in total volume. This is understandable since the particle volume does not change. Therefore every volume change
goes directly into a pore volume change. In PFC2D this is not entirely true because the particles overlap on compression which reduces the particle volume per area, see Figure 5.4.

Figure 5.4: Particle and pore volume reduction after compression.

The volume reduction for the particles remains small for most cases, therefore it’s assumed that equation (5.3) is valid. This equation is used in the coupled flow scheme Figure 5.2 to model the fully coupled flow in PFC2D.

5.2.2 Calculation of a stable time step

PFC2D selects a stable time step for the calculation. This step is valid for a particle assembly without pore fluid. The method used to calculate the time step is to estimate the natural frequency of each particle both for rotational and translational motion. A stable time step is always smaller than the period of the maximum natural frequency in the system. This leads to a critical time step for translational motion:

\[ t_{crit} = \frac{m}{\sqrt{k}} \]  

(5.4)

Where \( m/k \) is the minimum of particle mass divided by contact stiffness in the sample.

To estimate the critical time step for the situation with pore fluid, the stiffness of the sample with pore fluid has to be estimated. This can be done by assuming a square domain as shown in Figure 5.5.
Figure 5.5: Estimation of stiffness of a sample with pore fluid.

The initial total domain volume is $4r^2$ and if the upper side of the domain undergoes a displacement of $\Delta u$ then the total volume and pore volume (see previous section) decreases with $2r\Delta u$. According to equation (5.3), the increase in pore pressure due to the displacement $\Delta u$ is:

$$\Delta P = \frac{\Delta u}{2r} \frac{K_w}{n}$$

(5.5)

The force exerted on a particle in the $z$-direction can be calculated by integrating the pressure over the boundary of the particle while noting that although Figure 5.5 shows only a quarter of a particle in a domain, in reality there are more domains side by side and hence the integration can be carried out over half of the particle. Of course above and below the presented domain in Figure 5.5 there are also domains, but these are neglected because here the stiffness equivalent to one particle-particle contact is calculated. The force $F_z$ in $z$-direction becomes:

$$F_z = \int_{0}^{\pi} r\Delta P \sin \varphi d\varphi = 2r\Delta P$$

(5.6)

With equation (5.5) this becomes:

$$F_z = \frac{\Delta u K_w}{n}$$

(5.7)

Now, the fluid stiffness can be found $k_f = K_w/n$. Instead of a particle contact stiffness $k$, the stiffness is now $k+k_f$. Now the total stiffness is known, it can be substituted for the stiffness $k$ in the critical time step equation (5.4). It’s interesting to note that the mass of the fluid does not have to be taken into account in the equation for the critical time step, because the fluid has no mass in the code. The fluid simply gives rise to an external force but there is no extra inertia. Therefore the new critical time step $t_{*\text{crit}}$ can be calculated by substituting $k+k_f$ for $k$:
\[ t'_{\text{crit}} = \sqrt{\frac{m}{k + k_f}} = \sqrt{\frac{m}{k}} \left( \frac{1}{1 + \frac{k_f}{k}} \right) \]  

(5.8)

Therefore the new critical time step can be expressed in the old one:

\[ t'_{\text{crit}} = t_{\text{crit}} \sqrt{\frac{1}{1 + \frac{k_f}{k}}} \]  

(5.9)

The actual calculation of the critical time step in PFC2D is more complicated than shown here. PFC calculates an effective stiffness by summing the contribution of all contacts of a particle. Thus the contact stiffness \( k \) is not necessarily the contact stiffness given by the user. To calculate the factor in (5.9), this effective contact stiffness used by PFC2D is estimated by finding the smallest particle in the model, and use the given time step by PFC and the given particle mass to calculate the effective contact stiffness \( k \) with equation (5.4). With this value, equation (5.9) is used to calculate the critical time step for the case with fluid. This new time step will be used in the fully coupled calculations.

Simulations show that for sand like materials, with a user given contact stiffness in the order of 1GPa, the new critical time step \( t'_{\text{crit}} \approx 0.5 t_{\text{crit}} \), half that of the original PFC2D time step.

### 5.3 One-dimensional undrained compression test

To test the interaction of pore fluid with particles in case of fully coupled flow, a one dimensional undrained compression test is simulated. The test is modelled with a square-packed assembly of particles as shown in Figure 5.6.

![Simulation set-up of a one-dimensional compression test.](image)

Figure 5.6: Simulation set-up of a one-dimensional compression test.

Compression is assumed to be so quick that no flow is possible between domains. With this test, the increase of fluid pressure in the domains is determined, which can be verified with analytical results.
The test is made for a sample with a porosity $n=0.4$, a fluid bulk modulus $K_w=1.0\text{E}9\ \text{Pa}$ and a one dimensional elastic stiffness $E_{oed}=4.5\text{E}8\ \text{Pa}$. To model the correct contact stiffness in PFC2D, a particle normal stiffness of $9.0\text{E}8\ \text{N/m/m}$ was taken. Then the particle-particle stiffness is half of this stiffness resulting in a stiffness of $4.5\text{E}8\ \text{N/m/m}$, which is the same as $E_{oed}$. In the simulation, the horizontal stress is increased with steps of $2\text{E}4\ \text{Pa}$ until a total stress of $2\ \text{MPa}$ is reached.

Analytically, the total stress is separated in an effective stress and a fluid pressure according to Terzaghi’s principle:

$$\sigma = \sigma' + p$$  \hspace{1cm} (5.10)

And if the strains are small the following linear elastic relations can be used:

$$\sigma'_{xx} = -E_{oed} \varepsilon_{xx}$$

$$p = -\frac{K_w}{n} \varepsilon_{vol} = -\frac{K_w}{n} \varepsilon_{xx}$$  \hspace{1cm} (5.11)

Here pressure is taken positive, hence when the horizontal strain is negative on compression, both the effective stress and fluid pressure are positive.

In Figure 5.7, the effective horizontal stress and fluid pressures for the analytical case and PFC2D simulation with coupled flow are compared.

### One-dimensional undrained compression test

![Graph showing effective stress and fluid pressure during undrained compression test. Analytical results compared with PFC2D results.](image)

Figure 5.7: Effective stress and fluid pressure during undrained compression test. Analytical results compared with PFC2D results.
From the figure it can be seen that the simulation results agree reasonably well with the analytical results. For the effective stress the simulation results are almost identical to the theory, whereas for the fluid pressure, slight deviation occurs. This deviation is due to the implementation of equation (5.3) in the code which calculates the change of fluid pressure with pore volume. In the equation, the initial domain volume \( V_0 \) is used. However, in PFC2D, the initial volumes of the domains are not stored. This is also impossible to do, because in extensive simulation new domains are created while old ones are deleted when contacts are made or deleted. In the code, for the initial domain volume, the domain volume of the previous step is used, which leads to a small difference from the analytical results. In practice this difference will not influence the end result of the calculation. Also, for the total stress in the undrained compression test the difference between analytical results and the PFC2D simulation results are very small, see Figure 5.8. Therefore the current implementation is used in further calculations.

**One-dimensional undrained compression test**

![Graph showing total stress in the one-dimensional compression test. Analytical results compared with PFC2D simulation.](image)

Figure 5.8: Total stress in the one-dimensional compression test. Analytical results compared with PFC2D simulation.

### 5.4 One-dimensional consolidation with fully coupled particle pore-fluid interaction

After verifying the pressure change in the domain as a result of particle displacement in the previous section, a one-dimensional consolidation problem is simulated to see the performance of the fully coupled code for combined flow and deformation.

First, an initial state is created as shown in Figure 5.9.
As external pressure $\sigma_{ext}=2.0$ MPa is applied, while for the internal fluid a pressure of 1.8 MPa is applied. This fluid pressure is taken smaller than the applied external pressure to create an internal effective stress unequal to zero which makes it sure that all particles are in contact. With the fluid pressure of 1.8 MPa, the initial internal effective stress is 0.2 MPa. At the edges of the sample, two regions with fluid pressure zero are created which are boundary conditions for the flow calculation. The one-dimensional stiffness is chosen the same as for the undrained compression test in the previous section.

After the initial state has been created, the calculation is started by following the coupled flow scheme as was presented in Figure 5.2. After a flow step some fluid flows out of the sample decreasing the fluid pressure in the sample, in turn increasing the effective stress. This continues for a certain number of flow steps.

A sample was created having the same stiffness and fluid characteristics as in undrained compression test from the previous section. In total 8000 flow steps were performed. The analytical solution (2.19) for the one-dimensional consolidation equation has been used to compare the results. Here the consolidation coefficient $c_v$ has been chosen as in equation (2.18) which is for linear elastic one-dimensional deformation. The factor $m_s$ is then equal to $1/E_{oed}$. Results of the simulation and analytical calculation are shown in Figure 5.10. From the figure it can be seen that for this situation the fully coupled PFC2D simulation agrees well with the analytical results.
Figure 5.10: Results for fully coupled one-dimensional consolidation. PFC2D results compared with analytical results. On the horizontal axis is the horizontal distance along the sample where x=0 corresponds to the centre of the sample.

5.5 Computing time aspects

The one-dimensional consolidation simulation with fully coupled particle pore-fluid interaction took about 3.5 hours for 8000 flow steps on a Pentium III 550 MHz computer. The number of particles was 900. Therefore currently it seems not possible to use the fully coupled flow in for hydraulic fracturing calculations where at least several thousand particles are generated and the sample has an irregular shape which probably requires many more iterations to reach an equilibrium than the regular square packed sample used for the one-dimensional consolidation. Also domains are created and deleted when fractures appear complicating the matter even more.

However, it’s possible to use the developed fully coupling for the borehole alone and not for the surrounding domains. Then the domain volumes and pressure changes due to deformation only have to be recalculated for other domains except the borehole which requires much less computational effort. The advantage of a fully coupled borehole is that injection controlled hydraulic fracturing calculations can be made. When the borehole expands due to pressure increase the pressure drops and there is an equilibrium between fluid injection, fluid flow through the borehole and borehole expansion.
6 Conclusions

An implementation for fluid flow in the distinct element code PFC2D has been presented and verified for a number of cases. The fluid flow implementation agrees very well with analytical Darcy flow both qualitatively and quantitatively. Fluid flow is implemented in such a way that the user can give a porosity, permeability and bulk modulus for the fluid and can expect a behaviour very similar to the well known Darcy flow and consolidation without sample deformation. Quantitatively, the code agrees well for dense packed assemblies which are triangular in shape. These type of samples are most common if the random generation of particles in PFC2D is used.

Besides fluid flow, the interaction of pore fluid with particles has been described and modelled. Two types of interaction were presented. The first is a one-way interaction, where the pore pressures give rise to an external force on the particles thereby influencing the motion of the particles, but the particle movements don’t give a change in the pore pressures. The second is fully coupled flow where particle movement also causes pore pressures to change. Although the fully coupled flow case is more realistic, as was verified in one-dimensional consolidation with deformation and undrained compression test simulations, it is computationally very expensive.

For the hydraulic fracturing simulations it is recommended to use the one-way flow, since it’s computationally faster. This allows for hydraulic fracturing simulations to be made with acceptable computing times. The fully coupled flow can still be used in hydraulic fracturing simulations if only the borehole domain is modelled as fully coupled with all other domains remaining one-way coupled. Doing so enables the calculation of injection controlled fracturing calculations.
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