

# Simulation of triaxial compression test with *PFC3D*

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## 1 INTRODUCTION

Triaxial compression tests are often simplified as biaxial tests with rigid or flexible membranes in two dimensions (e.g. Iwashita & Oda 2002, Utili & Nova 2008, Wang & Leung 2008). Many researchers simulated true triaxial tests, in which cubic samples were fixed within flat rigid boundaries (e.g. Sitharam et al. 2002, Belheine et al. 2009, Salot et al. 2009). Nonetheless, these works demonstrated how rigid boundaries inhibit localization, causing significant non-uniformities in the stresses along the boundary.

Other researchers have simulated the effects of confining pressure by applying forces directly to the sample and allowing it to deform freely (Cheung & O’Sullivan 2008, Cui et al. 2008, O’Sullivan & Cui 2009, Wang & Tonon 2009, Baumgarten & Konietzky 2012). Since no boundary elements are used in this approach, the membrane-sample interaction cannot not be examined. Other approaches used bonded particles assembled in the shape of a sleeve (Cheung & O’Sullivan 2008, de Bono et al. 2013).

The main objective of this paper is to model the circumferential pressure acting on a flexible membrane by deformable independent wall elements to simulate triaxial testing. This approach enables updating the applied force on each membrane wall element under consideration of constant confining pressure and corresponding large deformations in the pre- and post-failure range.

## 2 DESIGN AND ANALYSIS

In this research, wall elements were used to provide the confining stress by a set of isolated walls to represent a deformable membrane.

The spatial positions of each wall element are determined by sets of *FISH* functions. In the parameter assignment file, the number of square wall units along the circumference is set to be 16, but can be enlarged to increase resolution. According to mathematical relation, the coordinates of the 16 vertices in each circle are also calculated. A basic triangular wall element is created based on 3 vertices in adjacent circles. With a fourth vertex, isosceles rectangular triangles are generated in pairs. Each pair of wall element forms one square wall unit. Circles of square wall units are stacked vertically to cover the entire sample to set-up the membrane (see Fig. 1a). The cylindrical membrane is longer than the sample to fully cover the model, and the outstretched parts are essential to keep the basic shape of the membrane. To simulate the confinement, wall servo commands are applied to each wall element. The model is reconstructed based on CT images. The samples consist of a coal matrix and organic inclusions. They are presented by green and red particles, respectively. The distributions of components are exactly inherited from real sample.

Testing was performed with confining pressures of 2.5 MPa, 5 MPa and 7.5 MPa respectively. For each wall element, the target force is calculated by the defined confining pressure multiplied by its area. The

simulated hydraulic pressures act on the normal direction of the walls. The coordinates of vertices are recorded during the test, which is essential for updating the confinement.

Before triaxial loading, a new wall servo command is applied to the loading platens together with the confinement, and the model reaches hydrostatic condition first. Then loading process acts with giving constant velocities of the loading platens. During the test, the macroscopic shape of the model (sample) deforms continuously and the side surfaces become uneven due to the failure pattern. Deviations from the target force lead to a translational velocity on the wall elements to achieve the desired condition. Consequently, nearly constant target forces are maintained by the movement of the wall elements.

A *FISH* function to update the contact force is activated every 1000 steps during the simulations, and the walls are either stretched or squeezed to maintain a closed membrane.

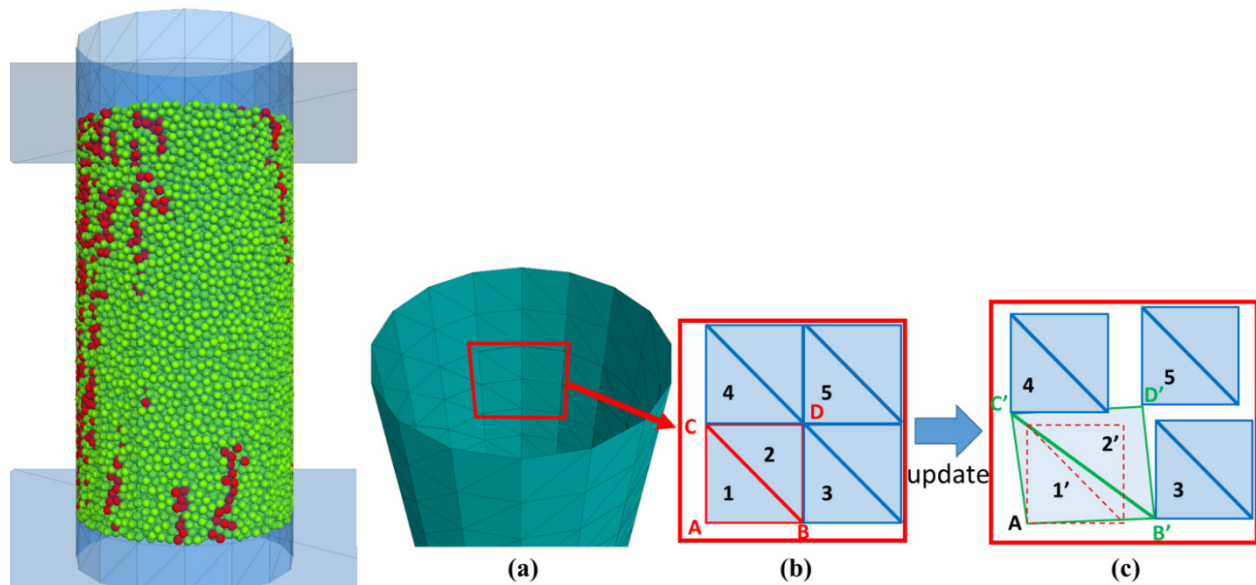


Figure 1. Sample modelling and theoretical flow chart of wall updating process.

See Figure 1: at the beginning, wall 1 and 2 consist of isosceles rectangular triangles as shown in Figure 1(b). After several steps, the walls move to new positions shown in Figure 1(c) and the triangles 1 and 2 in target are stretched and become triangles 1' and 2' with the new vertices B', C' and D'. All the wall units are adjusted according to the same rule, so that the confining structure is kept continuously updated to duplicate the deformed membrane. According to the applied *FISH* function, the area of each wall unit is calculated again after stretching or squeezing, and a new target force (equal to the confining pressure) is applied. By running these functions, the overall confinement remains constant even if significant deformations occur. The parameters of the wall-servo function affect the results. Therefore, the maximum velocity of the wall units should be smaller than the loading velocity, and the gain factor should also be adjusted. According to equilibrium, average vertical and horizontal stresses inside the sample should be consistent with applied boundary conditions. This criterion is used to validate simulation results.

### 3 RESULTS AND DISCUSSION

To test the developed routines, cylindrical models are loaded by constant velocities of the top and the bottom walls. A series of microscopic mechanical parameters were considered in the numerical model, such as bond elastic modulus ( $pb\_emod$ ), normal to shear stiffness ratio ( $kratio$ ), tensile strength ( $pb\_ten$ ), cohe-

sion ( $pb\_coh$ ) and friction angle ( $pb\_fa$ ). Some parameters have cross effects with each other on the macroscopic parameters, such as Poisson's ratio, peak strength and failure patterns. A specific calibration methodology has been proposed to overcome this cross dependency.

The use of confining wall elements causes an increase of the maximum differential stress. Triaxial simulation results are showed in Figure 2 for confining pressures of 2.5, 5.0 and 7.5 MPa.

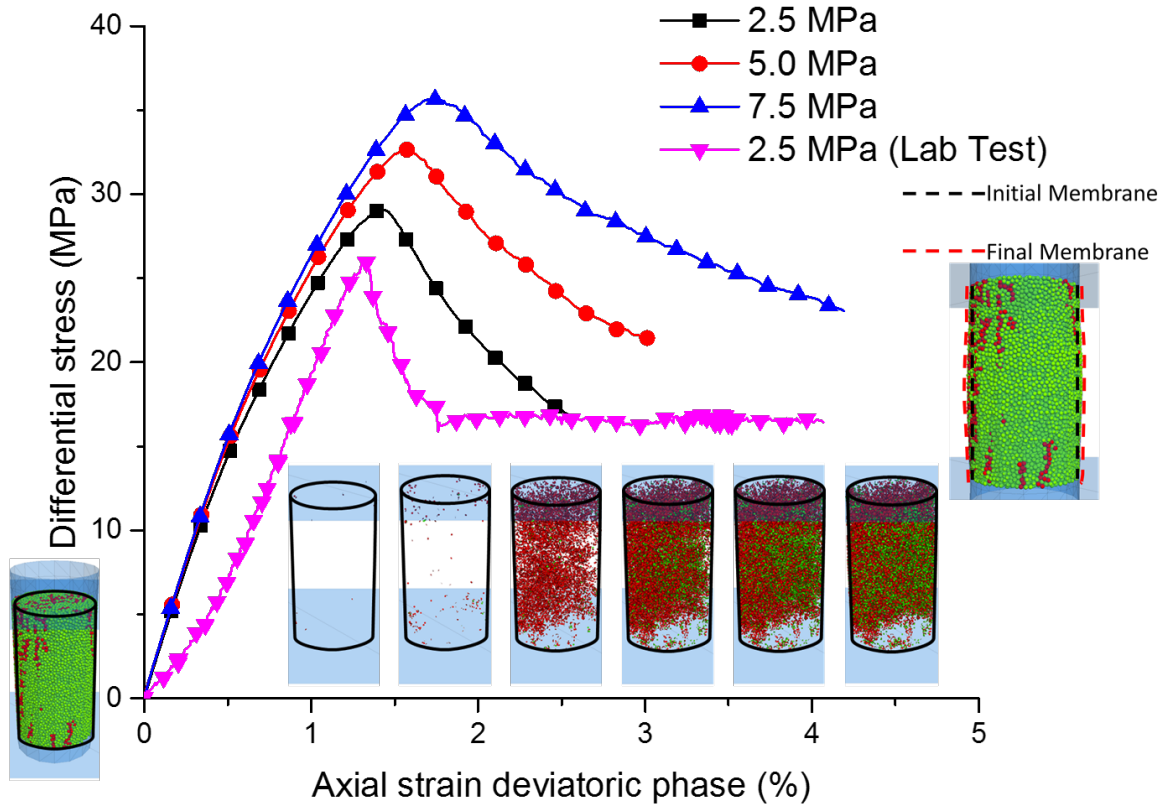


Figure 2. Simulated stress-strain curves and crack evolution for coal sample with 2.5 MPa confining pressure.

By using *PFC3D* (Itasca 2018) to simulate the triaxial compression tests, fracture initiation and propagation as well as failure pattern were analyzed based on coal samples tested in the lab.

The particle based models provided better insights into the micromechanical kinematics within the structure of coal samples. When the model was loaded in axial direction, contact forces increased at specific positions inside the model. The force chains are gathered around the composite boundaries. The force network showed that the stronger force chains developed nearly vertically in the central region before failure. The fractures were mostly initiated at the boundary between matrix and inclusions, and propagated along the boundary. The fractures extended along the direction of maximum principal stress inside the matrix and inclusions. Up to the peak stress state, continuous shearing caused anisotropic extension of force chain network. The collapse of main force chains led to the development of new force chains inside the model. Secondary contact force chains that carried smaller loads supported the major force chains that carried the majority of the applied deviator stress, this supports the statements of Cil & Alshibli (2014).

Compared with particle based membrane, the force chain network development shows a different propagation process in triaxial simulations compared to a flexible wall membrane. Higher contact forces were able to form at the membrane-sample interface during the simulations. Force chains developed at the boundary between different components and extended towards the wall elements. The general force chain magnitudes internally were proved to be larger than the ones in case of a particle membrane. Because the forces are applied in direction normal of each wall element, this might be attributed to a better stress localization along the membrane boundary. The force network pattern demonstrates the significant effect of wall elements on the contact force distribution.

The final fracture pattern was affected not only by the composite boundary itself but also by the confining pressure. With increasing confining pressure, the fractures expanded towards to the outer vertical boundary as mentioned before. This is because the confinement restrained the vertical propagation of fractures effectively, so the fractures deviated from the initial tracks.

The brittle-ductile transition scenario was also observed during the simulations with confinement. Please note, that the formation of some failure modes would be inhibited without a flexible membrane (e.g. Cheung & O'Sullivan 2008, Baumgarten & Konietzky 2012). The proposed scheme to simulate a soft membrane provides a better observation of the failure modes during deformation. The behavior inside the numerical samples was clearly observed by plotting the particle migration. The development of shear planes was observed with corresponding shear fracture network. The ductile behavior was suppressed by increasing confinement.

Figure 2 illustrates the stress-strain curves for different confining pressure and the crack distribution at 2.5 MPa confining pressure. Number of induced cracks increased drastically when axial stress reached the peak value. Which means large amount of micro fractures are generated in this stage, and macro fractures are formed. In the final stage of the simulations, there were more cracks in models with higher confining pressure. Because the lateral deformation was restrained: instead of generating macro fractures, diffuse micro cracks were generated. For a specific model, the peak strength increased with the increase of confining pressure. The pattern of inclusions has a great impact on the peak strength. The distributing of inclusions inside the coal matrix affected the fracture propagating paths.

#### 4 CONCLUSIONS

Triaxial tests are simulated in 3D with the particle-based DEM code *PFC3D* using a flexible membrane boundary. The flexible membrane is composed of triangular wall elements that form a cylindrical sleeve. In this paper, triaxial simulations are validated by comparing the stress-strain response and fracture pattern of coal samples tested in the laboratory via triaxial compression tests. Force chains evolved at the contacts at the membrane-sample interface, so the importance of realistic membrane boundary simulation is demonstrated and compared with other methods.

After calibrating the parameters, the results showed that DEM models can capture the expected macroscopic response for simulations with varying void ratio, confining stress and loading path without the need for model recalibration. The results showed that flexible wall membrane could replicate the boundary conditions better than rigid membrane or particle based membrane. It has been proven that the simulations have the ability to accommodate various failure modes. Different failure modes have been reproduced at different confining pressures by numerical simulations. Peak strength, failure pattern and deformation of a shear bands were observed at low confinement, and more volumetric contraction without formation of shear deformation zones were observed at higher confining pressure. Joint application of DEM and FDM to simulate stress-induced permeability evolution can be performed based on this modeling method.

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