PAPER • OPEN ACCESS

DEM (PFC^{3D}) numerical simulation of the influence of grain orientation on the strength of the Kimachi sandstone

To cite this article: G Smolnik 2019 *IOP Conf. Ser.: Earth Environ. Sci.* **261** 012047

IOP Conf. Series: Earth and Environmental Science **261** (2019) 012047 doi:10.1088/1755-1315/261/1/012047

DEM (PFC^{3D}) numerical simulation of the influence of grain orientation on the strength of the Kimachi sandstone

G Smolnik

Silesian University of Technology, Faculty of Mining and Geology, 2 Akademicka Street, 44-100 Gliwice, Poland

E-mail: grzegorz.smolnik@polsl.pl

Abstract. The set of the uniaxial compressive tests of differently oriented specimens of the Kimachi sandstone revealed the significant decrease of UCS values for some orientations of drilled cores. The laboratory obtained descriptions of behavior of Kimachi sandstone were bases for the DEM numerical modeling by means of ***PFC***^{3D}. The estimation of material constants of particles contacts models was based on the experimental results of uniaxial loading of rock specimens. The mimicked axial, circumferential and volumetric strains vs. axial stress relationships show good agreement with the experimentally obtained cures. The hypothesis of the possible influence of grain orientation on the strength of the Kimachi sandstone was then evaluated by creating models of specimens consisting of the so called "penny shaped" grains. The orientation of grains seems to prove its contribution in the changes of UCS values. The influence of angle of orientation of "penny shaped" grains can be, however, different for different inclination angle values, from very small decrease to significant drop of strength. Moreover the effect of inclination angle on strength variations is also affected by the confining pressure changes, as it is revealed from results of numerical analysis of conventional triaxial compression tests of models of specimens of Kimachi sandstone.

1. Particle Flow Code^{3D}

Particle Flow Code^{3D} is classified as a *discrete element code* based on the definition given by Cundall and Hart [1], since it allows finite displacements and rotations of discrete bodies (including complete detachment), and recognizes new contacts automatically as the calculation progresses. *PFC3D* can be viewed as a simplified implementation of the DEM because of the restriction to rigid spherical particles. (The general DEM can handle deformable polygonal-shaped particles.)

The calculation cycle in *PFC3D* is a timestepping algorithm that requires the repeated application of the law of motion to each particle, a force-displacement law to each contact, and a constant updating of wall positions. Contacts, which may exist between two balls, or between a ball and a wall, are formed and broken automatically during the course of a simulation. The calculation cycle is illustrated in figure 1. At the start of each timestep, the set of contacts is updated from the known particle and wall positions. The force-displacement law is then applied to each contact to update the contact forces based on the relative motion between the two entities at the contact and the contact constitutive model. Next, the law of motion is applied to each particle to update its velocity and position based on the resultant force and moment arising from the contact forces and any body forces acting on the particle. Also, the wall positions are updated based on the specified wall velocities. The calculations performed in each of the two boxes of figure 1 can be done effectively in parallel[2]

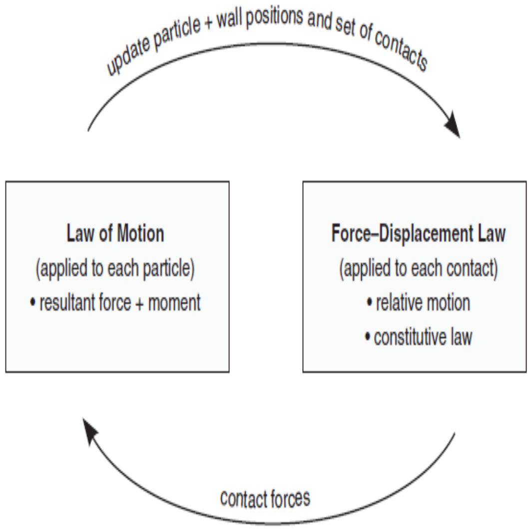

Figure 1. Calculation cycle in PFC^{3D}[2].

PFC3D provides a particle-flow model containing the following assumptions:

1. The particles are treated as rigid bodies.
2. The contacts occur over a vanishingly small area (i.e., at a point).
3. Behavior at the contacts uses a soft-contact approach where the rigid particles are allowed to overlap one another at contact points.
4. The magnitude of the overlap is related to the contact force via the force-displacement law, and all overlaps are small in relation to particle sizes.
5. Bonds can exist at contacts between particles.
6. All particles are spherical. However, the clump logic supports the creation of super-particles of arbitrary shape. Each clump consists of a set of overlapping particles that acts as a rigid body with a deformable boundary.

Among many possible uses of *PFC3D* , some of the applications are directly related to geo- or rock mechanics and exploit the ability of the program to model the interaction of many discrete objects, the large-strain capability (actually unlimited motion and/or separation), or the ability to treat the process of fracturing as the progressive breaking of discrete bonds. For instance the code has been applied for the analysis of

- mine caving: fracture, collapse, fragmentation and flow of rock blocks
- impact of objects composed of bonded particles: dynamic breakage
- seismic response and collapse of structures composed of beams represented by arrays of bonded particles
- fundamental studies of granular materials: yield, flow, volume changes, etc.
- fundamental studies of solids, represented by bonded assemblies of particles: damage accumulation, fracture and acoustic emission.

The broad scope of possible applications and details of the analyses preformed both by Itasca scientists and engineers worldwide can be traced, for instance, in [3, 4 , 5].

2. Granular model of Kimachi sandstone and the results of numerical simulations

The sample of synthetic material in PFC^{3D} is represented as an assembly of spherical particles. The granular model of the Kimachi sandstone specimen was prepared based on the laboratory obtained properties of both the rock and the specimen itself. The model of specimen is a right circular cylinder of 50 mm diameter and 100 mm height. Figure 2 shows the initial assembly of particles of aspect ratio 2:1. It contains 2686 balls with radii ranging uniformly from 0.625 to 1.25 mm (2.5 times the real

Kimachi sandstone grain radii). The density and porosity of Kimachi sandstone was also mimicked in a model of rock specimen.

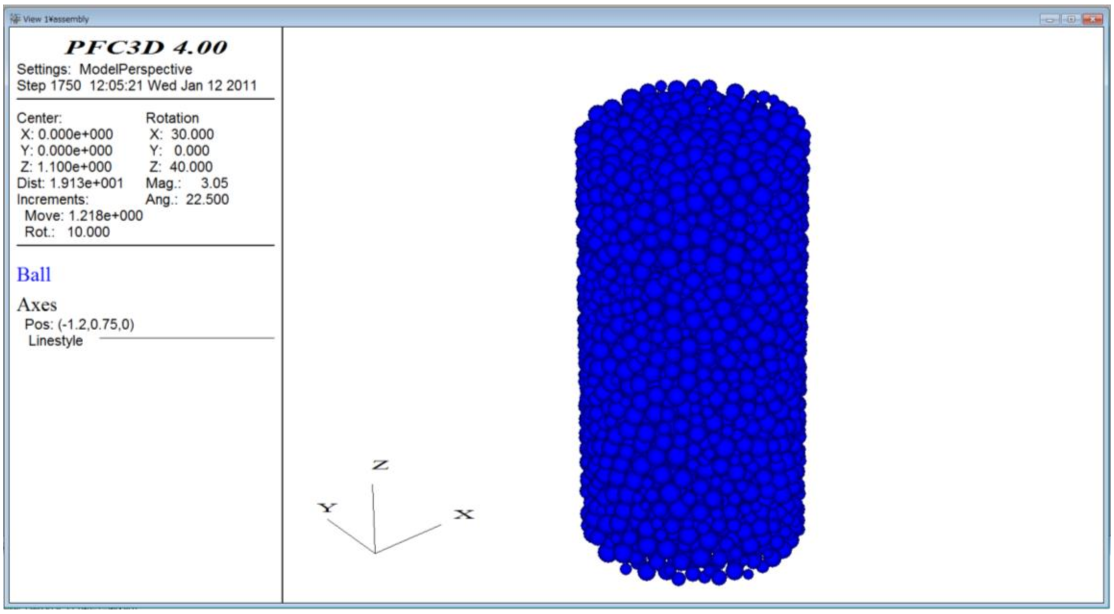

Figure 2. Initial stage of Kimachi sandstone PFC3D numerical model.

The cylindrical sample was then used to simulate a uni- and triaxial tests by confining a specimen comprised of a compacted particle assembly. The top and bottom walls simulate loading platens, and the lateral cylinder wall simulates the confinement experienced by the sample. The sample is loaded in a strain-controlled fashion by specifying the velocities of the top and bottom walls. During all stages of the test, the radial velocity of the cylindrical confining wall is controlled automatically by a numerical servomechanism that maintains a constant confining stress within the sample. The stresses and strains experienced by the sample are determined in a macro-fashion by summing the forces acting upon walls and tracking the relative distance between appropriate walls, respectively.

The estimation of material constants of particles contacts models (stiffness and friction coefficients, tensile and shear strengths) was based on the experimental results of uniaxial loading of rock specimens. The parallel bond contact model was chosen and shear and normal strength values varied as a function of spatial location. The values of properties of both balls and parallel bonds used in numerical simulations are summarized in table 1.

Table 1. Material constants of balls and parallel bonds

ρ (kg/m^3)	pb_k_n (GPa/m)	pb_k_s (GPa/m)	*pb_nstrength* (MPa)	*pb_sstrength* (MPa)	*friction coef.* -	*pb_radius* -
2230	3150	2625	50-110	60-120	0.3	1

ρ – density, pb_k_n – parallel bond normal stiffness, pb_k_s – parallel bond shear stiffness, *pb_nstrength* – parallel bond normal strength, *pb_sstrength*– parallel bond shear strength, *friction coef.*- friction coefficient of ball surface, *pb_radius* – radius multiplier such that parallel-bond radius equals this multiplier times the minimum radius of the two bonded balls

The mimicked axial, circumferential and volumetric strains vs. axial stress relationships show good agreement with the experimentally obtained cures (figure 3).The example set of results of three laboratory tests (specimen number 4, 10 and 12) of uniaxial loading of Kimachi sandstone specimens were presented. The Unconfined Compressive Strength of selected cases were neither the maximum nor the minimum ones - the “average” response of Kimachi sandstone was selected to be mimicked by numerical simulation. The hypothesis of the possible influence of grain orientation on the strength of the Kimachi sandstone was then evaluated by creating models of specimens consisting of the so called “penny shaped” grains. The orientations (inclinations) of “penny shaped” clusters of grains towards loading direction in models of specimen were changed in subsequent models but the values of material contact models constants were preserved for all the numerical models of specimens, to be the same as in the “initial” model of Kimachi sandstone.

The details of creation of clusters and the appearance of the PFC3D model of rock with penny shaped grains are presented in figures 4 and 5, respectively. The lattice consisting of 25 cells was prepared, the dimensions of single “brick” were 10 mm×10 mm×2.5 mm, so the cell height was equal to maximum ball diameter, width and depth of it were four times the maximum single particle diameter. The total number of 40 layers of grid of that kind was placed one by one from the bottom to the upper side of the specimen and all the balls with centers initially located inside any single cell were put together to create single clump.

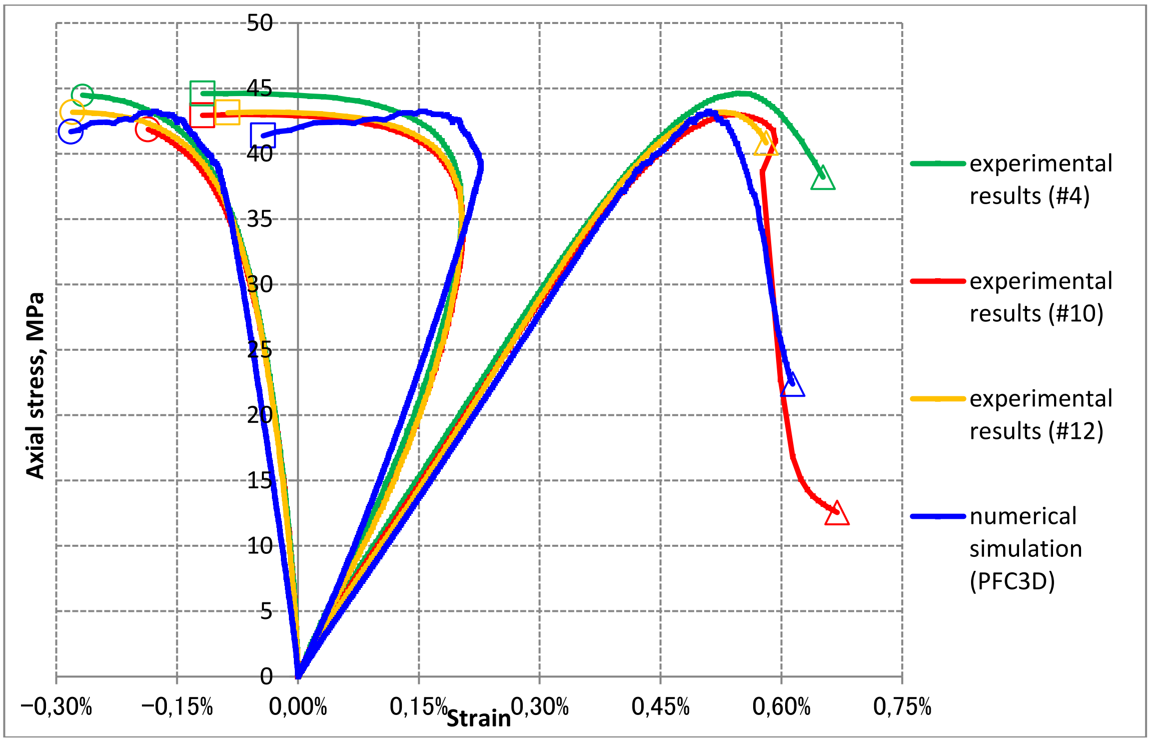

Figure 3. Axial (△), volumetrical (□) and circumferential (○) strain versus axial (vertical) normal stress curves as results from both laboratory testing and numerical simulations.

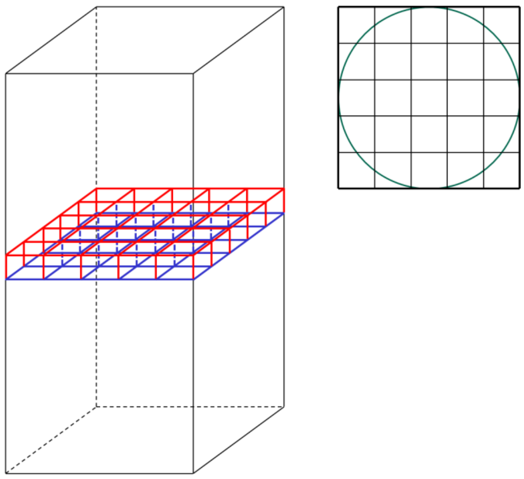

Figure 4. The approach for creating clumps of balls. The single lattice layer (left), top view of grid superimposed on specimen base (right).

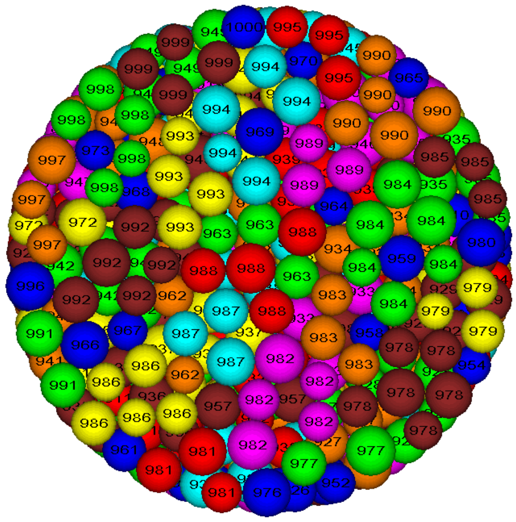

Figure 5. Top view of the specimen model with horizontally oriented clumps.

For horizontal inclinations of single layer of grid – one thousand clumps consisting of two to seven balls were created (some isolated special clumps of single ball also remained).Side view of the specimen consisting of horizontally oriented clumps and enlarged central part of it are presented in figure 6. The colors and numbers indicate the clumps; the height of the lattice (equal to maximum particle diameter) enhances some distortion to perfect flatness of clumps – easily visible in presented view.

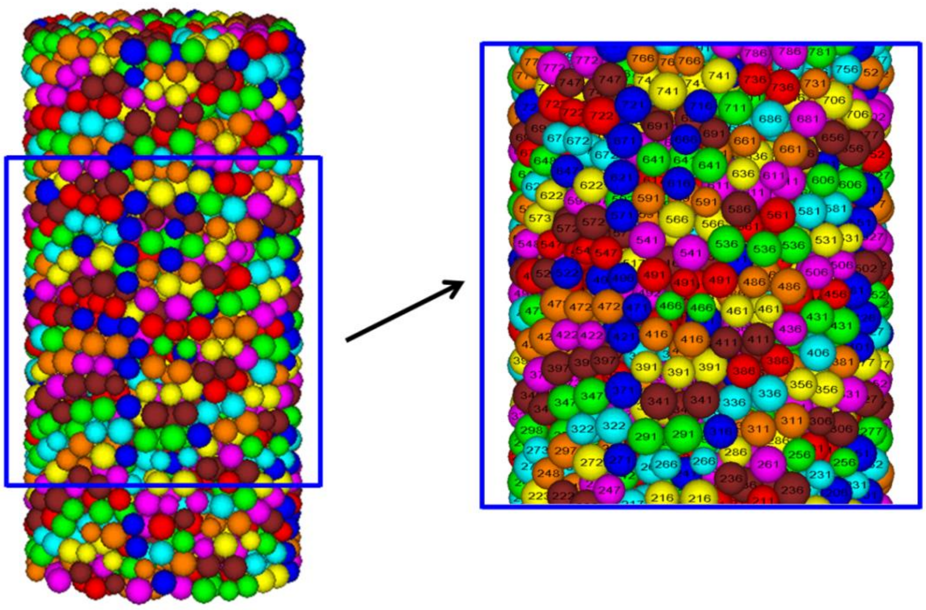

Figure 6. General view of specimen with horizontally oriented clumps (left), enlarged view of central part (right).

IOP Conf. Series: Earth and Environmental Science **261** (2019) 012047 doi:10.1088/1755-1315/261/1/012047

The grain orientation changes were subsequently simulated by introducing the change of inclination angle α of the lattice layers as can be seen in figure 7. The inclination angle α was assumed to be 30, 45, 60 and 90 degrees. The side view of middle part of the model of specimen with clumps created for 45 degrees inclination angle is shown in figure 8.

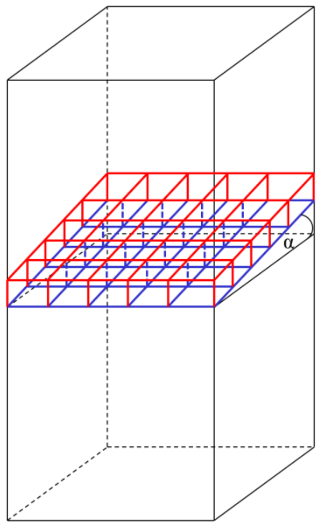

Figure 7. Mesh for creating inclined penny shaped grains.

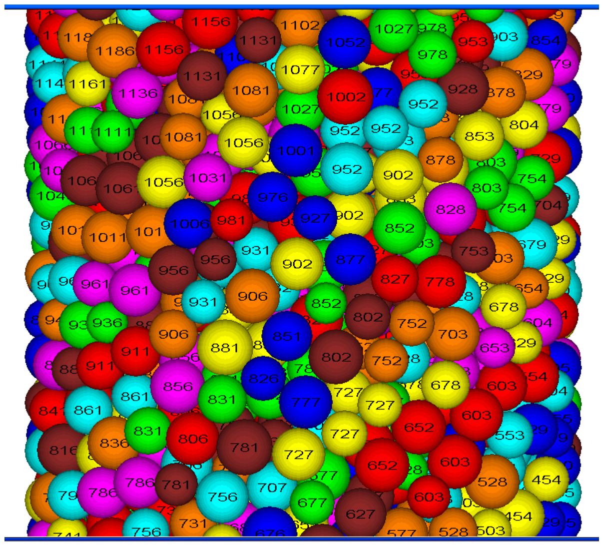

Figure 8. Side view of central part of granular model with clumps oriented at 45 degrees angle.

The results of the numerical simulations of uniaxial compressive loading of the specimens are presented in figure 9. There are significant differences of UCS values for different orientation of clumps, ranging from about 67 MPa to 53 MPa. The most dramatic drop occurred for α angle equal to 60 degrees.

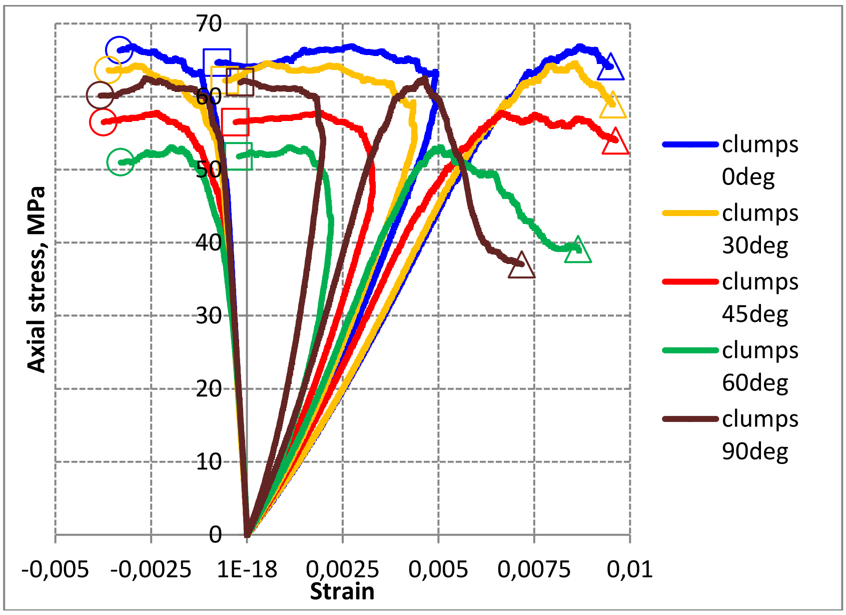

Figure 9. Axial (△), volumetrical (☐) and circumferential (◯) strain versus axial (vertical) normal stress curves for specimens consisting of clumps oriented at α angle equal to 0, 30, 45, 60 and 90 degrees.

The pattern of changes of Unconfined Compressive Strength of numerical models of specimen with inclined penny shaped grains (figure 10) agrees with well know variability of UCS values for anisotropic rocks like slates [6, 7].

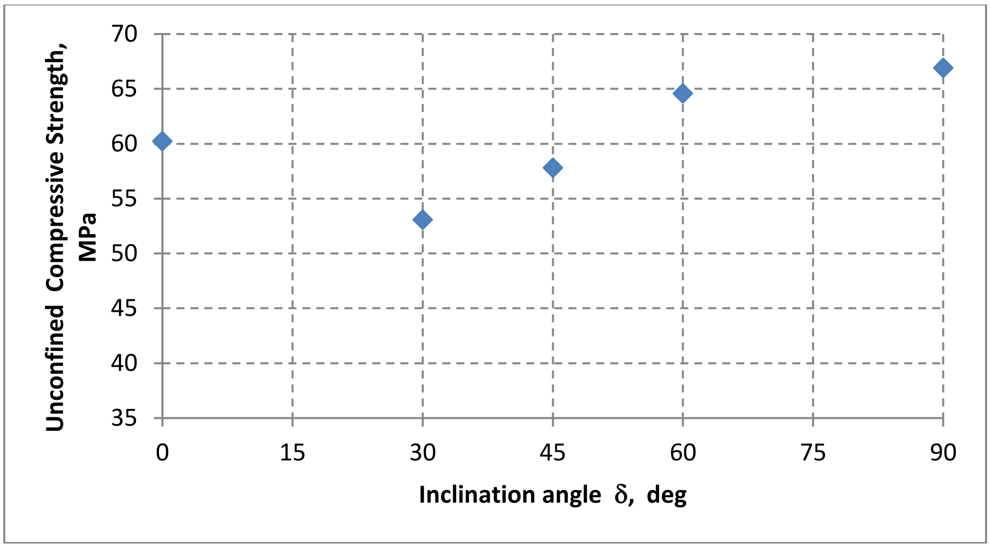

Figure 10. Uniaxial Compressive Strength of models of specimens created with penny shaped grains oriented at angle δ to the vertical direction.

Inclination angle δ is equal to 90°-α to present data in a more common form, where inclination angle is measured to vertical plane.

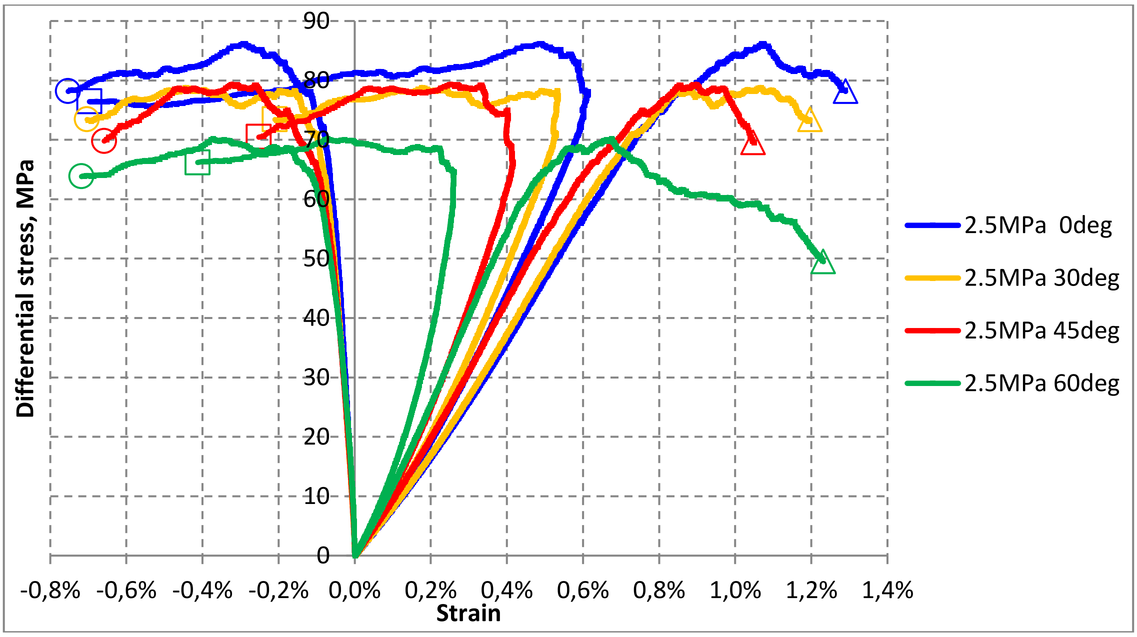

Figure 11. Axial (△), volumetrical (□) and circumferential (○) strain versus differential stress curves for specimens consisting of differently oriented clumps loaded in triaxial compression conditions under 2.5 MPa confining pressure.

Strength of granular models is strongly affected by even small confining presser under conventional triaxial compression conditions (figure 11 and 12). Confining pressure equal to just 2.5MPa gives increase of strength (differential stress at failure) of a range of 15-20 MPa for different orientation of grains.

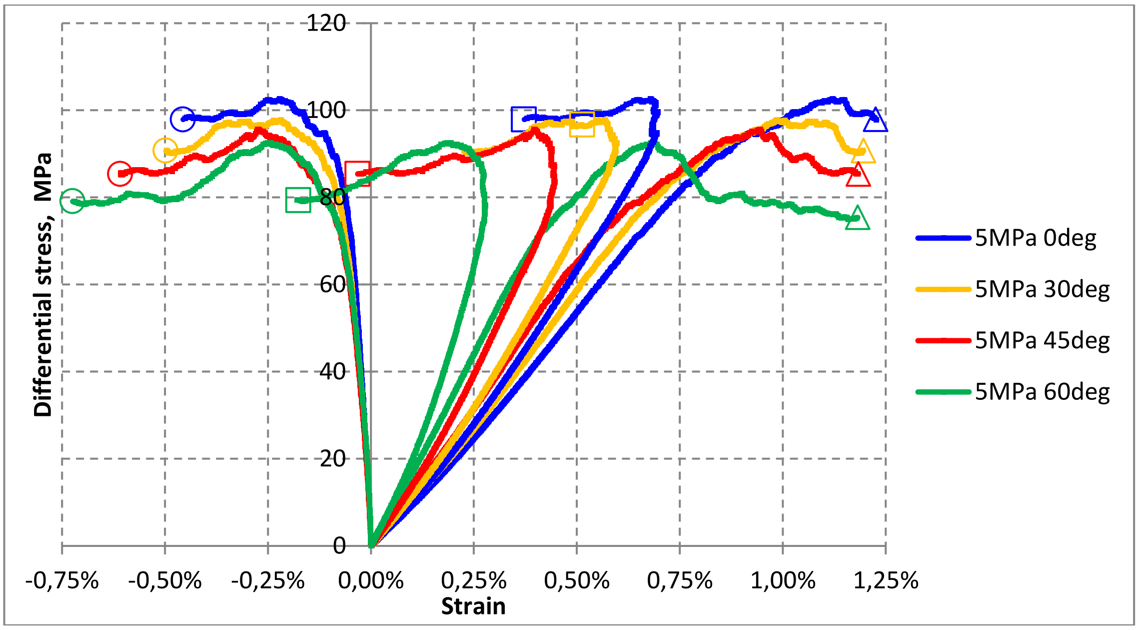

Figure 12. Axial (△), volumetrical (□) and circumferential (○) strain versus differential stress curves for specimens consisting of differently oriented clumps loaded in triaxial compression conditions under 5 MPa confining pressure.

Although the difference in strength for 0 and 60 degrees orientations remains significant, maximum differential stress for 30 and 45 degrees inclined clumps is almost the same.

Increase of confining pressure value to 5 MPa causes consequent increase in strength but the variances between differently oriented sets of clumps seems to diminish for all selected angles of inclination of penny shaped grains.

3. Conclusions

The uniaxial compressive tests of differently oriented specimens of the Kimachi sandstone revealed the significant decrease of UCS values for some orientations of drilled cores. As the existence of the non-spherical “penny-shaped” grains was confirmed by detailed petrographic studies the hypothesis of the influence of grain orientation on the strength variations was suggested. In order to verify the validity of the hypothesis DEM PFC3D numerical model of a sandstone was built and the simulations of compressive tests performed. The laboratory obtained descriptions of behavior of Kimachi sandstone and extensive experimental tests results of uniaxial loading of specimens of that rock made the estimation of material constants of particles contact models possible.

The first stage of the analysis was successful as the mimicked axial, circumferential and volumetric strains vs. axial stress relationships show good agreement with the experimentally obtained cures. The hypothesis of the possible influence of grain orientation on the strength of the Kimachi sandstone was then evaluated by creating models of specimens consisting of the so called “penny shaped” grains. The orientation of grains seems to prove its contribution in the changes of UCS values. The influence of angle of orientation of “penny shaped” grains can be, however, different for different inclination angle values, from very small decrease to significant drop of strength. Moreover the effect of inclination angle on strength variations is also affected by the confining pressure changes, as it is revealed from results of numerical analysis of conventional triaxial compression tests of models of specimens of Kimachi sandstone.

As Kimachi sandstone was chosen few years ago by the Japanese rock mechanics and geosciences researchers as one of a new “reference rocks” which will be extensively used in different kinds of tests in order to discover and/or prove new features of rocks behavior the results of the study presented can be regarded as a contribution towards the goal of better understanding of the behavior of this important rock.

4. References

[1] Cundall P A and Hart R 1992 *J. Engr. Comp.* **9** 101
[2] Itasca Consulting Group, Inc. 2008 *PFC^{3D}(Particle Flow Code in 3 Dimensions), Version 4.0.* (Minneapolis: ICG)
[3] Proc. of the 1st Int. PFC Symp. on “*Numerical Modeling in Micromechanics via Particle Methods’* (6-8 November 2002 Gelsenkirchen) ed H Konietzky (Lisse: A.A. Balkema)
[4] Proc. of the 2nd Int. PFC Symp. on “*Numerical Modeling in Micromechanics via Particle Methods’* (28-29 October 2004 Kyoto) ed Y Shimizu et al (Leiden: A.A. Balkema)
[5] Proc. of the 4th Itasca Symp. on Applied Numerical Modeling “*Applied Numerical Modeling in Geomechanics - 2016’* (7-9 March 2016 Lima) ed P Gomez et al (Minneapolis: Itasca International Inc.)
[6] Twiss R J and Moores E M 1993 *Structural Geology* (New York: W H Freeman and Company)
[7] Brown E T, Richards L R and Barr M V 1977 *Proc. Conf. Rock Engng. Newcastle upon Tyne* pp 33-51

Acknowledgments

Author is grateful to Dr Manabu Takahashi who was his host researcher during his post-doc post at Geological Survey of Japan of the National Institute of Advanced Industrial Science in Tsukuba near Tokyo, Japan and made the analysis presented in the paper possible and to Dr Hyuck Park who conducted the uniaxial compressive tests of Kimachi sandstone.