

## Usability Assessment of Different Contact Models for Modelling the Failure Behaviour of Sedimentary Rocks Under Unconfined Stress Conditions

*Sedimanter Kayaçların Tek Eksenli Gerilme Koşullarında Yenilme Davranışlarının Modellenmesi için Farklı Temas Modellerinin Kullanılabilirliklerinin Değerlendirmesi*

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### ABSTRACT

The methods applied in rock material and rock mass studies related to rock mechanics have begun to differentiate with computational and software technology development in recent years. Particle Flow Code software, which is based on the discrete element method, is used in many studies on rock mechanics. Using Particle Flow Code, rock behaviour under different stress conditions can be modelled and analysed in both two and three dimensions. Rocks can be presented by an assembly of disks in two dimensions and spherical particles in three dimensions. These particles are bonded to each other by contact models with different micro-mechanical properties. Model failure occurs as a result of the fracturing with the rupture of these bonds. Using parameters such as density, strength, deformation, which can be defined as the mathematical expression of the natural properties of rock samples, a representative models can be created by following multi-stage calibration procedure and used for different research purposes. In order to have a representative model, chosen contact models should be mimic the failure behaviour of the rock material. For this purpose, calibrated models were created for both PBM (Parallel-bonded model) and FJM (Flat-jointed model) using the experimental results of the unconfined compressive strength test of Hawkesbury sandstone in the laboratory. In the calibration phase, the results obtained from the models were compared against micromechanical data obtained from the laboratory experiments such as elasticity modulus, uniaxial compressive strength, tensile strength, and Poisson ratio. Results were evaluated by considering the displacement vectors, force chains, and crack parameters in terms of resolution and representativeness of the failure behaviour. The results of PBM and FJM model results were similar for displacement vector direction and orientation and distribution of the forces effective in breaking the bonds which is force chain. However, in terms of fracture resolution and localization, FJM provides detailed results, of which could be very useful for comprehensive studies.

**Keywords:** Hawkesbury sandstone, failure behavior, parallel-bond model, flat-joint model, Particle Flow Code

**ÖZ**

*Kaya mekaniği ile ilgili hem kaya malzemesi hem de kaya kütlesi ölçeğinde yapılan çalışmalarda uygulanan yöntemler son yıllarda gelişen hesaplama ve yazılım teknoloji ile birlikte farklılaşmaya başlamıştır. Ayrık elemanlar yöntemini temel alan Particle Flow Code yazılımı kaya mekaniği ile ilgili birçok çalışmada kullanılmaktadır. Particle Flow Code ile kayaların farklı gerilme koşulları altındaki davranışları hem iki hem de üç boyutlu olarak modellenilebilir ve analiz edilebilir. Kayalar iki boyutta diskler, üç boyutta ise küresel tanecikler kullanılarak oluşturulurlar. Bu tanecikler ise birbirlerine farklı mikro mekanik özelliklere sahip olan temas modelleri ile bağlanırlar. Oluşturulan bu bağların kopması ile meydana gelen çatlakların sonucu olarak modelde yenilme meydana gelir. Kaya örneklerinin doğal özelliklerinin sayısal ifadesi olarak tanımlanabilecek yoğunluk, dayanım, deformasyon gibi parametreler kullanılarak çok aşamalı kalibrasyon adımlarının ardından oluşturulan modeller farklı gerilim koşulları altındaki kaya davranışına yönelik çalışmalar yapılabilmektedir. Kalibre edilmiş ve temsil edici bir modele sahip olabilmek için seçilen bağ modelinin kaya malzemesinin yenilme davranışını tam olarak yansıtması gerekmektedir. Bu amaç doğrultusunda Hawkesbury kumtaşına ait olan tek eksenli sıkışma dayanımı deneyi sonuçları kullanılarak hem PBM (Paralel-bonded model) hem de FJM (Flat-jointed model) için birer tane olmak üzere iki tane kalibre edilmiş model oluşturulmuştur. Kalibrasyon aşamasında modellerden elde edilen sonuçlar, elastisite modülü, tek eksenli basınç dayanımı, çekme dayanımı ve Poisson oranı gibi laboratuvar deneylerinden elde edilen mikromekanik verilerle karşılaştırılmıştır. Sonuçlar yer değiştirme vektörleri, kuvvet zincirleri ve çatlak çözünürlükleri parametreleri dikkate alınarak değerlendirilmiştir. PBM ve FJM kullanılarak oluşturulan modeller yer değiştirme vektörleri ve kuvvet zincirleri açısından benzerlik göstermiştir. Bununla birlikte çatlak çözünürlüğü açısından FJM, PBM'e göre çatlak çözünürlüğü ve lokalizasyonu açısından daha detaylı ve kapsamlı veri sunması nedeniyle yenilme davranışının analiz edilmesinde ve sedimanter kayalara yönelik modelleme çalışmalarında kullanılabilirlik açısından öne çıkmaktadır.*

**Anahtar kelimeler:** *Hawkesbury kumtaşı, yenilme davranışı, parallel-bond model, flat-joint model, Particle Flow Code*

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**INTRODUCTION**

The mechanical behavior of rocks is fundamentally controlled by their microstructure and inherit properties on a material scale. Especially on laboratory tests, obtained results are a simplified numeric representation of rock's internal composition and structure such as mineralogy, grain size, pores, and flaws, which are the main reasons for the crack formation that leads to the ultimate failure of rock material. Considering this complex and heterogonous structure of the rock material, it has been defined that rocks act like a cemented granular material of complex-

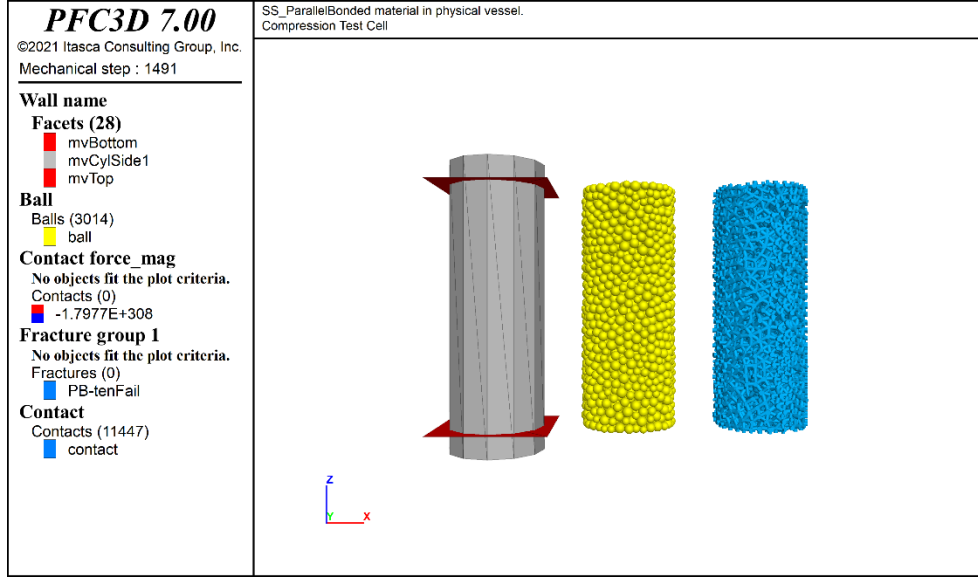
shaped grains in which both the grains and the cement are deformable and may break to develop a representative numerical model for rock behavior on both micro and macro scale (D. O. Potyondy and Cundall, 2004). As a result of this approach, the bonded-particle model (BPM), which depicts the behavior of rocks under different stress conditions in both two and three dimensions. BPM has been extensively used in rock mechanics investigations since it was proposed (Castro-Filgueira et al., 2017; Hazzard et al., 2000; Mas Ivars, 2010; Vallejos et al., 2016). Since then, the BPM has provided a scientific instrument to

investigate the micro-mechanisms that couple to produce complex macroscopic behaviors. Many detailed studies have been carried out to understand the cracking phenomena within the rocks to explain the failure evolution (Bieniawski, 1967a, 1967b; Hallbauer et al., 1973; Kranz, 1979). Experimental investigations propound that most of the compression-induced cracks nucleate around the rocks inherent natural weak spots like grain boundaries, cavities, gaps, pores. In order to model the behavior of rocks with numerical analysis methods, BPMs should be able to mimic the rock's complex structure under different stress conditions. Based on this theory, a general-purpose distinct-element modeling framework Particle Flow Code (PFC), was developed and distributed by ITASCA (D. O. Potyondy, 2017, 2018; D. O. Potyondy and Cundall, 2004). PFC models simulate the interaction and movement of finite-sized particles under Newton's laws of motion. During the simulation, particles can be moved independently depending on their bond status, translate, and rotate. It is also possible to create granular models using the same fundamental approach except for strong bonds between particles. Fundamentally, the PFC simulates the movement of particles and their mechanical interaction at pair-wise contacts. These particles could be defined as disks in 2D and spheres in 3D with finite mass and surface, named balls. Also, walls that are linear segment in 2D and triangles in 3D are used to both create assembly and perform numerical laboratory tests such as frictionless loading platens. A bonded assemble can be created by bonding particles with defining a specific contact model. A simple PFC model includes balls for rock grains, walls to create assembly implement fractures, apply load and contacts to create a bonded assembly (Figure 1). There

are several key points and assumptions that need to know about BMP;

1. Each particle (Circular in 2D, Spherical in 3D) is a rigid body and has a finite mass.
2. The particle can move, translate or rotate independently from each other. Particles only interact with each other on contact points.
3. Bonds between particles can carry the load and break depending on their micromechanical parameters, which represent the rock material's macroscopic properties.
4. Newton's laws apply during the model simulation.

The most crucial component of a PFC model is the contacts. Contacts are the bodies that bond balls and create a bonded assembly with their own unique micro mechanic properties and carry the load at a certain specific point until they break. A new crack called fracture is formed in every bond breakage depending on the increase in load. The collection of fractures form of failure planes. Therefore, it is crucial to define contact model properties which store in the "Contact Model Assignment Table (CMAT)" to mimic rock failure under load. In rock mechanics modeling studies, sedimentary rocks are preferred in terms of their less heterogeneous structure and predominant composition of similar minerals. For this purpose, Hawkesbury sandstone test results were used to create the PFC model and investigate the performance of PBM and FJM to represent the failure behavior of the rock material. Hawkesbury sandstone has been studied extensively in the literature and there is open-source access to the experimental results (Ord et al., 1991; Pells, 2004, 2017; Ranjith et al., 2012). In order to evaluate the usability and performance of the models created by using PBM and FJM under unconfined stress



**Figure 1.** Main components of PFC model; i) Walls (on left, red, and grey), ii) Balls (center, yellow) and iii) Contacts (right, blue).

**Şekil 1.** PFC modelinin temel bileşenleri; i) Duvarlar (solda, kırmızı ve gri), ii) Tanecikler (ortada, sarı) ve iii) Bağlar (sağda, mavi).

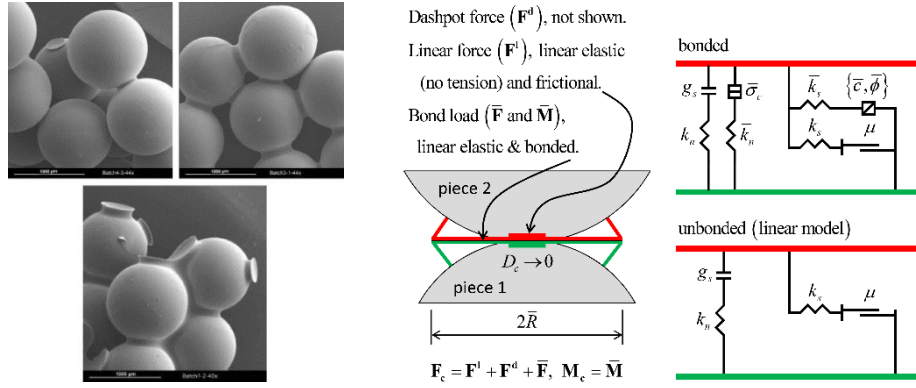
conditions, a complex calibration process has been followed. To evaluate the usability and performance of PBM and FJM under unconfined stress conditions, a complex calibration process has been followed for both contact models separately. The behavior of these models was investigated in detail after achieving a calibrated state.

## DEFINITION OF CONTACT MODELS

### Parallel-Bonded Model

The fundamental theory behind the PBM is the mechanical behaviour of a finite-sized piece of cement-like material between two contacting pieces. This behaviour was represented by epoxy cementing the glass beads (Figure 2). A parallel bond can be described as a set of elastic springs having normal and shear

stiffnesses, uniformly scattered over a cross-section lying on the contact plane and centred at the contact point. These cross-sections are rectangular in 2D and circular in 3D. These springs behave in parallel with the springs of the linear component. As a result of motion at the contact due to stress change following the creation of the contact leads to a developing of force and moment within the bond material. This force and moment exploit on the two contacting pieces and can be related to maximum normal and shear stresses acting within the bond material at the bond perimeter. If any of the maximum normal or shear stresses acting over the bond will exceed the bond strength, the parallel bond breaks, and its effect is removed from the model in terms of force, moment and stiffness PBM provides the



**Figure 2.** SEM image of the picture epoxy-cemented glass bead sample (Holt et al., 2005), Behavior and rheological components of the PBM-Based with inactive dashpots (D. O. Potyondy & Cundall, 2004).

**Şekil 2.** Epoksi ile çimentolanmış cam kürelerinin SEM görüntüsü (Holt et al., 2005), Etkin olmayan PBM'in davranışı ve reolojik bileşenleri (D. O. Potyondy & Cundall, 2004).

behaviour of both frictional and bonded interfaces. The frictional interface is infinitesimal, linear elastic with no tension, and carries force. The bonded interface is a finite-size, linear elastic and carries moment (D. O. Potyondy & Cundall, 2004).

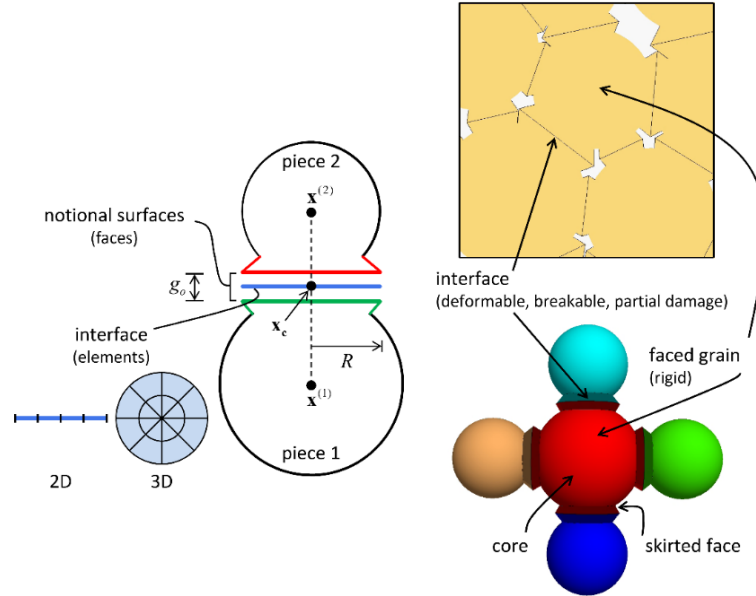
#### Flat-Jointed Model

The FJM provides the macroscopic behaviour of a finite-size, linear elastic, and either bonded or frictional interface that may maintain partial damage. FJM was introduced by (D. O. Potyondy, 2012) and its simplified illustration is given in Figure 3. FJM imitates the microstructure of angular, interlocked grains, which can be pretty similar to marble microtexture and structure; after all, usage of FJM is not limited to marble-like rocks and could be implemented for all types of rocks. The FJM interface is discretized into different elements. Each element can be bonded or unbonded, and the breakage of each bonded element contributes partial damage to the interface. A

model created by using FJM behaves like a linear elastic until the strength limit exceeds. At that critical point, bond breaks, and the model behaves like unbonded, linear elastic, and frictional with slip in terms of Columb limit on the shear force. Every element of the model carries force and moment and follows the force-displacement law and the model's response obeys that depiction.

#### Calibration of Synthetic Rock Material

The creation of the representative synthetic rock model (SRM) is one of the biggest challenges of numerical studies in rock mechanics. A calibrated model should mimic the complex behaviour of rock under different stress conditions and produce a reliable response. The very first step of creating SRM is the calibration process. The main requirement for the calibration process is to have extensive knowledge about e about rock



**Figure 3.** Simplified illustration of FJM (Flat-joint model) (left) and material (right) (D. O. Potyondy, 2012).

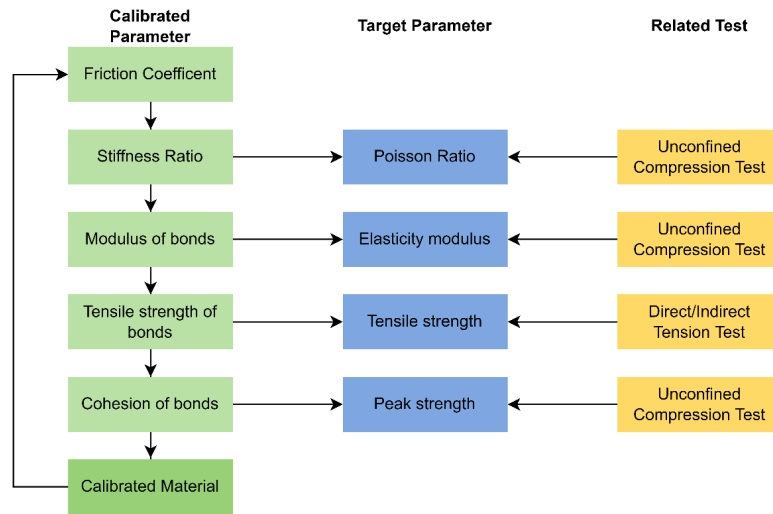
**Şekil 3.** FJM (solda) ve malzemenin (sağda) basitleştirilmiş illüstrasyonu (D. O. Potyondy, 2012).

behaviour and the results of laboratory tests like unconfined compressive strength, direct/indirect tension, and triaxial under different confining pressures. There are multiple micro-mechanical parameters in PFC that differ depending on the chosen contact model. The primary purpose in the calibration phase is to have a model which can achieve the results obtained from the laboratory experiments. A representative model is tried to be obtained by constantly changing the micro-mechanical parameters, a simple approach of continuous back-engineering. The most crucial micromechanical parameters are the modulus, cohesion, tension strength, friction angle, and the stiffness of the bonds. Both BPM and FJM have similar micro-mechanical parameters.

There are multiple suggested calibration flow for the PFC model (Castro-Filgueira et al., 2016; D. Potyondy, 2019; D. O. Potyondy and Cundall, 2004; Schöpfer et al., 2009; Wu and Xu, 2016). The calibration steps used in this study are given in Figure 4, considering the proposed flow by other studies.

### NUMERICAL MODELLING OF HAWKESBURY SANDSTONE

In this study, experimental results of Hawkesbury sandstone were used (Ord et al., 1991; Pells, 2004; Ranjith et al., 2012). Hawkesbury sandstone is a homogeneous medium-grained sandstone from Gosford, New South Wales, Australia, and it is typically massive and predominantly consists of sub-



**Figure 4.** The flow chart of the calibration process.

**Şekil 4.** Kalibrasyon işleminin akış şeması.

angular quartz grains. In addition, the target mechanical parameters used in this study can be listed as follows; elasticity modulus is 1.01 GPa, unconfined compressive strength is 36.51 MPa, and tensile strength is 3.40 MPa. Detailed and complex calibration steps were followed to achieve the mechanical properties derived from laboratory results. Calibrated micro-mechanical parameters for both PBC and FJMs are given in Table 1 and comparison with laboratory results are given in Table 2 and Figure 5. UCS tests were applied by using pre-defined FISH scripts embedded within the PFC. Load was controlled with 0.0003 mm/s constant strain rate in the vertical direction during the test until the occurrence of the ultimate failure. The tests were continued until a 20% drop in the peak strength value of the model throughout the simulation. In addition, stress and deformation values and the number and type of cracks occurring in the model during the experiment were recorded for further analysis. Similarly, direct tension tests were performed to calibrate the model tension behaviour. In order to apply direct tension on

the model, grip grains were defined for balls on the top and bottom of the model to behave like a wall to apply tension. As in UCS, tension was controlled with 0.0003 mm/s constant strain rate and continued until a 20% drop in the tension strength.

#### Sensitivity Analysis

In order to ensure that the results of the models are irrespective of the numerical resolution, a detailed sensitivity analysis was carried out on the model samples. In this regard, five model packings presented in Figure 6 are generated in the same dimension (D: 54 mm, L: 135 mm) but in different particle numbers (24222, 7193, 3014, 1550, 629 respectively) and are subjected to same compressive loading condition. It is worth noting that all models have the exact same micro-mechanical parameters provided in Table 1. At the end of this simulation process, the second, third and fourth model samples present very similar mechanical properties for both methodologies (PBM and FJM) (Table 3).

**Table 1.** Micromechanical parameters of PBM and FJM used in model calibration.**Tablo 1.** Model kalibrasyonunda kullanılan PBM ve FJM ait mikromekanik parametreler.

Parameters	Contact Model	Parameter	Calibrated Values
pbm_coh	PBM	Cohesion	18.0e6
fjm_coh	FJM	Cohesion	40.0e6
pbm_bemod	PBM	Effective modulus	0.63e9
pbm_emod	PBM	Effective modulus	0.63e9
fjm_emod	FJM	Effective modulus	1.30e6
pbm_fa	PBM	Friction angle	0
fjm_fa	FJM	Friction angle	0
pbm_fric	PBM	Friction coefficient	0.4
fjm_fric	FJM	Friction coefficient	0.4
pbm_krat	PBM	Stiffness ratio	1.5
fjm_krat	FJM	Stiffness ratio	1.5
pbm_ten	PBM	Tensile strength	3.70e6
fjm_ten	FJM	Tensile strength	5.20e6

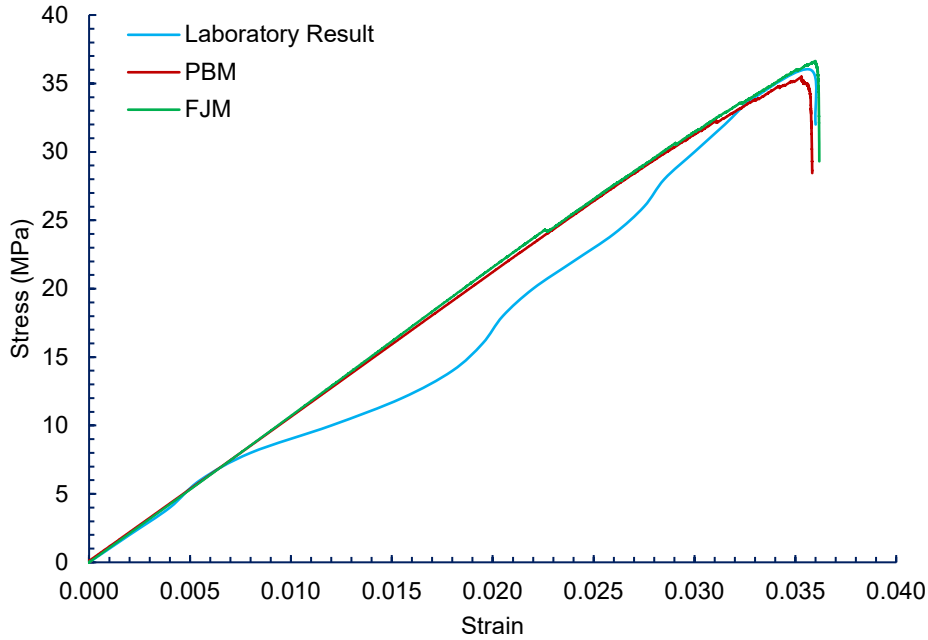
**Table 2.** Comparison of laboratory and model results.**Tablo 2.** Laboratuvar ve model sonuçlarının karşılaştırılması.

Parameters	Laboratory	PBM	FJM
Peak strength (MPa)	36.51	35.49	36.64
Tensile strength (MPa)	3.40	3.41	3.46
Modulus of elasticity (GPa)	1.01	1.04	1.06

**Table 3.** Results of the sensitivity analysis.**Tablo 3.** Hassasiyet analizlerinden elde edilen sonuçlar.

Model	# Balls	Peak Strenght (MPa)	Tensile Strenght (MPa)	Modulus of Elasticity (GPa)
Laboratory		36.51	3.40	1.01
PBM-1	24222	39.87	3.68	1.11
PBM-2	7193	37.16	3.55	1.08
PBM-3	3014	35.49	3.41	1.04
PBM-4	1550	37.74	3.62	1.04
PBM-5	629	32.67	3.46	1.01
FJM-1	24222	42.34	3.53	1.14
FJM-2	7193	36.79	3.77	1.09
FJM-3	3014	36.64	3.46	1.06
FJM-4	1550	35.18	3.75	1.04
FJM-5	629	23.28	3.50	1.02





**Figure 5.** Stress-strain graphs of the Hawkesbury sandstone and the models.

**Şekil 5.** Hawkesbury kumtaşı ve modellerin gerilim-birim deformasyon grafikleri.

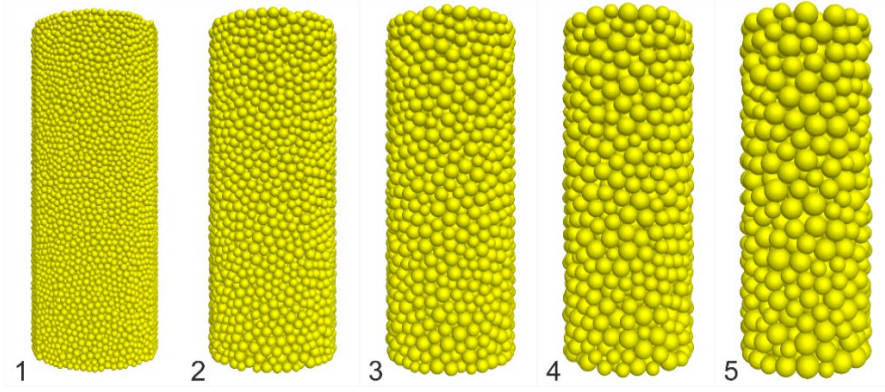
Therefore, to keep the optimum computational time during the simulations, the third model sample with 3014 particle numbers are selected to carry out the analyses in this study.

## RESULTS

In order to assess the usability of different contact models to represent sedimentary rock behaviour under unconfined stress conditions, two models based on PBM and FJM having different micro-mechanical parameters were calibrated to produce the similar macro mechanical properties of Hawkesbury sandstone. The comparison of the stress-strain curves obtained from the unconfined compressive strength tests between numerical predictions and laboratory measurements are given in Figure 6. Obtained results confirm that a successful calibration phase was carried out in terms of elasticity modulus, peak strength, tensile strength, and Poisson ratio. Numerical

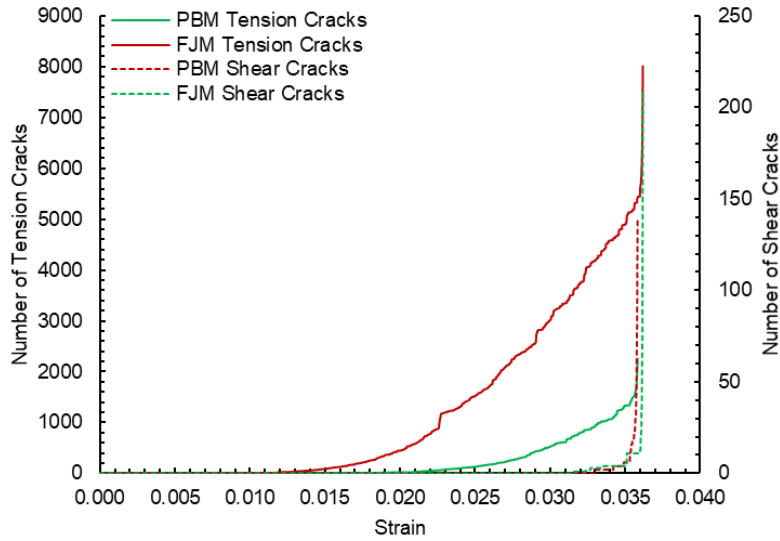
models successfully reproduce the behaviour of rock material. However, at this point, due to the nature of numerical approaches and limitations, it is not possible to mimic the localized stress drop during the initial phase of the test which is also known as crack closure. To create a model to reproduce this behaviour, the mechanical properties of the minerals of the rock should be defined separately, and the resolutions of the model should be increased drastically. Defining the mechanical properties of minerals is a broad subject that needs to be studied entirely separately. Also, increasing the resolution of the model requires having a tremendous computational effort. In this study, every model consists of around 3000 balls and 12000 contacts with around 6-12 hours of computational time. Increasing the resolution causes the computation time to increase in parabolic, up to 120 hours or more.

Shear and tension cracks were recorded from the PBM and FJM at frequent intervals for comprehensive evaluation (Figure 7). The crack numbers given in Figure 6 represent the ruptures that occur as a result of the load applied to model exceeding the strength value



**Figure 6.** Models used in sensitivity analyses (1: 24222 particles, 2: 7193 particles, 3: 3014 particles, 4: 1550 particles, 5: 629 particles).

**Şekil 6.** Hassasiyet analizlerinde kullanılan modeller (1: 24222 tanecik, 2: 7193 tanecik, 3: 3014 tanecik, 4: 1550 tanecik, 5: 629 tanecik).



**Figure 7.** The number of tension and shear cracks in PBM and FJM under unconfined compressive loading.

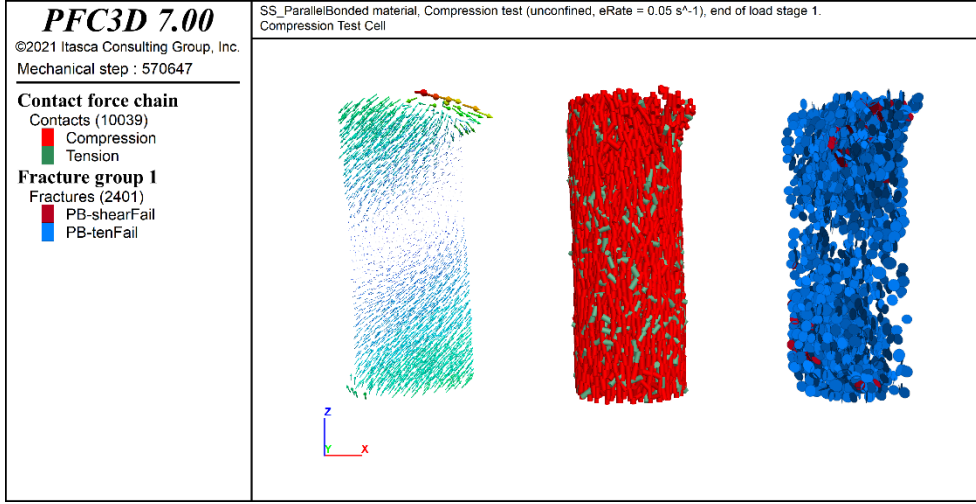
**Şekil 7.** Tek eksenli yükleme koşullarında PBM ve FJM'de meydana gelen çekme ve makaslama çatlaklarının sayısı.

of the bonds. The behaviour of the bonds depending on the applied load is given in the second heading of the paper. Depending on the mechanical definitions of PBM and FJM, their behaviours under load are utterly different from each other. Even if the models are calibrated in terms of elasticity modulus, peak strength, tensile strength, and Poisson ratio, they must also represent failure behaviour derived from the stress-strain response. The crack numbers and types can give an idea to the readers about the mechanisms driven in the sample during loading. This parameter can also be used to compare the failure behaviour of the sample and the model, given in Figure 5. As it can be seen in the laboratory results, failure principally occurred under the effect of tension cracks formed in the direction parallel to the loading direction. Therefore, the number of cracks obtained from the models are mainly of tensile cracks. The total number of cracks formed in the PBM is 2401 and for the FJM is 8218, respectively. The ratio of tensile cracks to the total number of cracks is 94.2% in PBM and 97.5% in FJM. Meanwhile, the number of shear cracks is 5.8% of the total cracks in PBM and 2.5% in FJM emerged mainly prior to the failure. This result can be considered as a numerical expression of failure under the control of tension cracks. In addition, it is seen that from the force chains, models were failed under the dominance of the compressional forces. However, there is no distinctive difference between the two models in terms of force chains.

#### **DISCUSSION AND CONCLUSIONS**

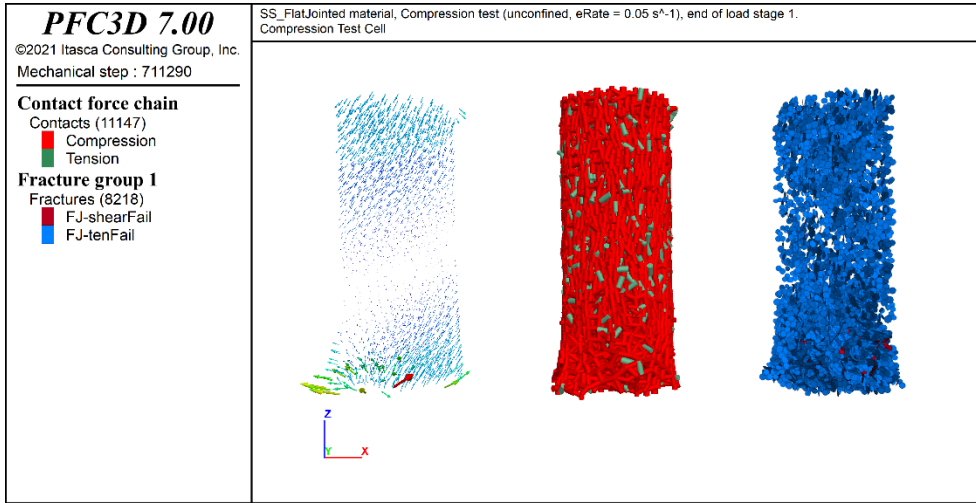
PBM and FJM yielded results consistent with mechanical parameters obtained from laboratory results, such as elasticity modulus, peak strength, tensile strength, and the Poisson ratio. On the other hand, these results

are not sufficient to decide the usability of the contact model in terms of modelling the failure behaviour of sedimentary rocks under unconfined loading conditions. In order to distinguish the PBM and FJM, the model results were analysed in more detail in terms of post-failure conditions, which are given in Figure 7 and Figure 8, respectively. It can be stated that the displacement vectors in both models created by using PBM and FJM are predominantly in the same direction and orientation, with some minor differences between them. This behaviour shows that both models successfully simulate the displacements within the sample. Accurate determination of displacement vectors is crucial because it is a parameter that is frequently used in many small and large-scale geological and geotechnical studies, from tunnelling to hydraulic fracturing (Chiu et al., 2014; Moffat et al., 2015; Verde and Ghassemi, 2015). The extreme displacement values on the top of the PBM and the bottom of the FJM, which can be seen from Figures 8 and 9, emerged due to the rapid free movement of the particles prior to the ultimate failure of the model. In PFC models, the particles move freely until they reach the domain when the bonds forming the model are broken. As a result of the unconfined compression test performed with axial loading, it is seen that both PBM and FJM bonds are carried stress along the entire model surface. It is another critical phenomenon that is essential for evaluating the model response against stress change and variations. The bonds between the spherical particles that form up the model are broken if they are subjected to stress above the strength value. As a result of this particular event, a new fracture occurs. The collection of fractures lead to the failure of the model.



**Figure 8.** Post failure status of the model created by using PBM-Based; a) Displacement vectors, b) Force distributions in bonds, c) Types of cracks.

**Şekil 8.** PBM kullanılarak oluşturulan modelin yenilme sonrası görünümü; a) Yer değiştirme vektörleri, b) Bağlardaki kuvvet dağılımları, c) Çatlakların türleri.



**Figure 9.** Post failure status of the FJM; a) Displacement vectors, b) Force distributions in bonds, c) Types of cracks.

**Şekil 9.** FJM'in yenilme sonrası görünümü; a) Yer değiştirme vektörleri, b) Bağlardaki kuvvet dağılımları, c) Çatlakların türleri.

Tracking fracturing events within the model allow to determine the crack closure, crack initiation and crack closure points which are essential to evaluate the failure behaviour and understand the response of the rock against loading and stress variations which could be very useful for different research topics related to earth sciences. Therefore, the bond model preferred.

In this numerical study, which was carried out using the results obtained from the unconfined compression strength experiments of Hawkesbury sandstone, the usability performance of models (PBM and FJM) was analysed considering the failure behaviour of sedimentary rocks in terms of number of the cracks, displacement vectors and force chains.

The performances of PBM and FJM provide similar results for displacement vectors and force chain parameters. However, FJM provides a more detailed fracturing data structure rather than PBM, exceeding four times in terms of crack resolution. Due to this difference, it has been concluded that FJM is more beneficial for modelling the failure behaviour of sedimentary rocks. In addition to obtained results, it is thought that it would be beneficial to perform laboratory-scale experiments with acoustic emission measurements to study in detail the relationship between cracking in the sample and fracturing in the model and to analyse the performance of the contact models under different stress conditions by performing triaxial compression strength tests under different lateral pressure conditions.

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