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Simulating spalling with a flat-jointed material

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1 INTRODUCTION

The Swedish Nuclear Fuel and Waste Management Company (SKB) is developing a methodology for long-term storage of nuclear spent fuel in an underground repository in compact crystalline rock (SKB 2011). The repository design calls for the placement of the spent nuclear fuel in copper canisters in vertical 1.8 meter diameter boreholes of 8 meter length. It is likely that the stress redistribution around the excavations, along with the thermal load from the decaying spent nuclear fuel, will induce stress at the borehole walls that is greater than the rock mass strength, and thereby produce an excavation damaged zone (EDZ) in which hydromechanical and geochemical modifications may induce significant changes in flow and transport properties. The mechanical characteristics of this EDZ must be understood to evaluate its impact on repository performance.

Our understanding of the damage process can be enhanced by performing in-situ testing. The Äspö Pillar Stability Experiment (Andersson & Martin 2009, Andersson et al. 2009) is one such in-situ test. The experiment was performed in Äspö diorite and consisted of drilling two vertical 1.75 meter diameter boreholes of approximately 6 meter length separated by a one meter pillar. The pillar was loaded by a combination of excavation-induced stresses and heating of the surrounding rock. In this way, the tangential stress on the pillar boundary could be controlled in a very precise manner.

In competent crystalline rock, the EDZ takes the form of spalling on the excavation boundaries, whereby a localized damage region forms at the location of the maximum tangential stress. Spalling begins with small rock chips forming on the boundaries of the excavation. In the APSE experiment, the chips ranged in size from a finger nail to approximately $0.1\ \mathrm{m}^2$. Larger chips formed beneath the small chips. The chips are tangential to the hole wall and are believed to have formed in tension. The spalling region evolves into a v-shaped notch as the tangential stress increases with crushing and/or shearing at the notch tip, suggesting that the chip-forming process is suppressed at the notch tip. In the APSE experiment, rock mass yielding occurred when the tangential stress on the hole boundary reached 59% of the unconfined-compressive strength of the intact rock. Changes in the tangential stress of approximately one MPa beyond this threshold expanded the extent of rock mass yielding, indicating that a distinct stress level threshold needs to be reached before the rock yields.

Our understanding of the damage process can also be enhanced by numerical modeling. This paper summarizes the results of a study to evaluate the ability of the *PFC* (Itasca 2018) flat-jointed material model to simulate spalling (Potyondy 2019). Both 2D and 3D flat-jointed Äspö diorite materials were created, and their response during direct-tension and compression tests was studied. The material behavior is described in Section 2. Borehole models of a cylindrical hole in an infinite medium were created and used to approximate the conditions in the APSE experiment. The behavior of the borehole models is described in Section 3. Conclusions of this study are provided in Section 4.

2 FLAT-JOINTED MATERIALS

The flat-joint contact model provides the macroscopic behavior of a finite-size, linear elastic, and either bonded or frictional interface that may sustain partial damage. A flat-jointed material mimics the microstructure of angular, interlocked grains. We refer to the balls of a flat-jointed material as faced grains, each of which is depicted as a spherical core and a set of skirted faces (see Fig. 1a). The flat joint model formulation is given in Potyondy (2018).

Both 2D and 3D flat-jointed materials to represent Äspö diorite were created and subjected to direct tension and compression tests. These materials match the Young's modulus, direct-tension strength, unconfined-compressive strength, and peak strength at 7-MPa confinement. The crack-initiation stress is too low, the crack-damage stress is too high, and the Poisson's ratio is too low. No attempt was made to match the crack-initiation and crack-damage stresses. Attempts to increase the Poisson's ratio were unsuccessful. The material behavior during these tests is like the brittle behavior of compact rock (Potyondy 2015), with the exception that transgranular cracking occurring within and across grains during the compression tests is absent. In compact rock under near-zero confinement, axial splitting occurs, and with increased confinement, shear fractures form. These behaviors are exhibited by the 2D flat-jointed material but appear to be absent in the 3D flat-jointed material. Although there is extensive dilation after the crack-initiation point in the 3D flat-jointed material, localizations associated with axial splitting and shear-fracture formation are absent; instead, the deformation field remains homogeneous.

Microstructural validity describes whether the grain faces overlap one another; a flat-jointed material has a valid microstructure if and only if the faces of each grain can be connected to the grain center with no overlap. A valid microstructure is physically realizable — i.e., a physical replica of such a material could be constructed. An invalid microstructure may produce useful behavior, and as such, its use can be justified. For the present modeling effort, microstructurally valid and invalid instances of the flat-jointed material that match the Äspö diorite properties listed above were created (see Fig. 1b). The microstructurally valid 2D material was selected for the borehole models because it is physically realizable. The microstructurally invalid 3D material was selected for the borehole models because the microstructurally valid 3D material was deemed to be unrealistic, having a very small amount of cement with excessively long cement bridges that overlap across bonded regions and microproperties approximately 3.5 times larger than their corresponding macroproperties to compensate for the fact that the interfaces do not fully cover the ball surfaces. This suggests that the 3D flat-jointed material may not be well-suited to model a compact rock like Äspö diorite and may be better suited to model a more porous rock like a sandstone. The *PFC3D* bonded-block model that represents the rock as a bonded collection of rigid polyhedral blocks with an initial porosity of zero may be better suited to model compact rock.

The flat-jointed material exhibits a size effect with modulus and peak compressive strengths increasing with increasing specimen resolution (number of grains across the specimen width) until a representative volume is reached. There is no size effect for the tensile strength and Poisson's ratio. The representative volumes for the 2D and 3D materials correspond with specimen resolutions of approximately 25 and 50, respectively. For the 3D material, the values reach approximately 92% of their asymptotic values at a resolution of 20. The specimen resolution is the controlling parameter — i.e., the same response is obtained by either varying the specimen size while keeping the average grain diameter constant or varying the average grain diameter while keeping the specimen size constant.

3 BOREHOLE MODELS

Both two- and three-dimensional borehole models of a cylindrical hole in an infinite medium, have been developed. The two-dimensional models approximate the conditions for the Kirsch solution (long excavation with a circular cross-section in a medium subject to biaxial stress), whereas the three-dimensional models are quasi 3D, meaning that plane-strain conditions are enforced on a plane normal to the hole axis and the model thickness in this direction is small relative to the hole diameter (with approximately four grains through the thickness). These borehole models include *PFC* models (both 2D and 3D) and a coupled *FLAC3D-PFC3D* model. The coupled model allows greater hole resolution (number of grains across the hole diameter) to be obtained in the near-borehole region.

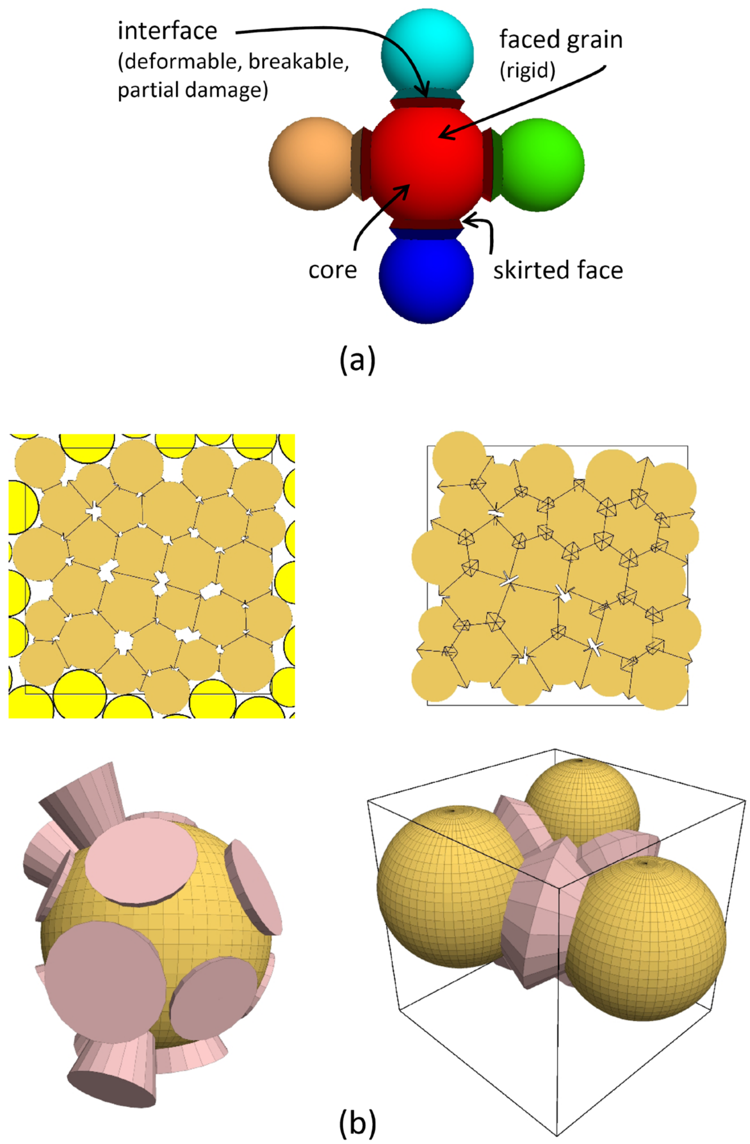

Figure 1. (a) Flat-jointed material; and (b) microstructural characteristics of the four materials (left: microstructurally valid, right: microstructurally invalid) that match the properties of Äspö diorite.

The borehole models *approximate* the conditions in the Äspö Pillar Stability Experiment. After excavation of the hole, the maximum tangential stress reaches 165 MPa according to the Kirsch solution, but only reaches 128 MPa according to a stress analysis accounting for the drift and both holes. A set of coupled borehole models is constructed for which the material grain size is varied to produce models with a range of hole resolutions. The displacement field is compatible across the coupling interface (see Fig. 2a), and when the models are run elastically, the excavation-induced displacements provide a good match to the Kirsch solution for all hole resolutions. The damage increases with increasing hole resolution, with gradual delineation of a spalling zone and two damage lobes (see Fig. 2b). These damage features become more clearly delineated as grain size is reduced from 55 to 9 mm. This is approaching the grain size of Äspö diorite (which ranges from 0.1 to 5 mm). It is expected that the model response will best match the rock behavior when the average grain size of the model is equal to that of the rock; therefore, the general damage characteristics are studied for the model with the 9-mm grain size. This model has 718,000 balls with a total run time of 48 hours on a PC with an Intel Xeon CPU at 3.4 GHz.

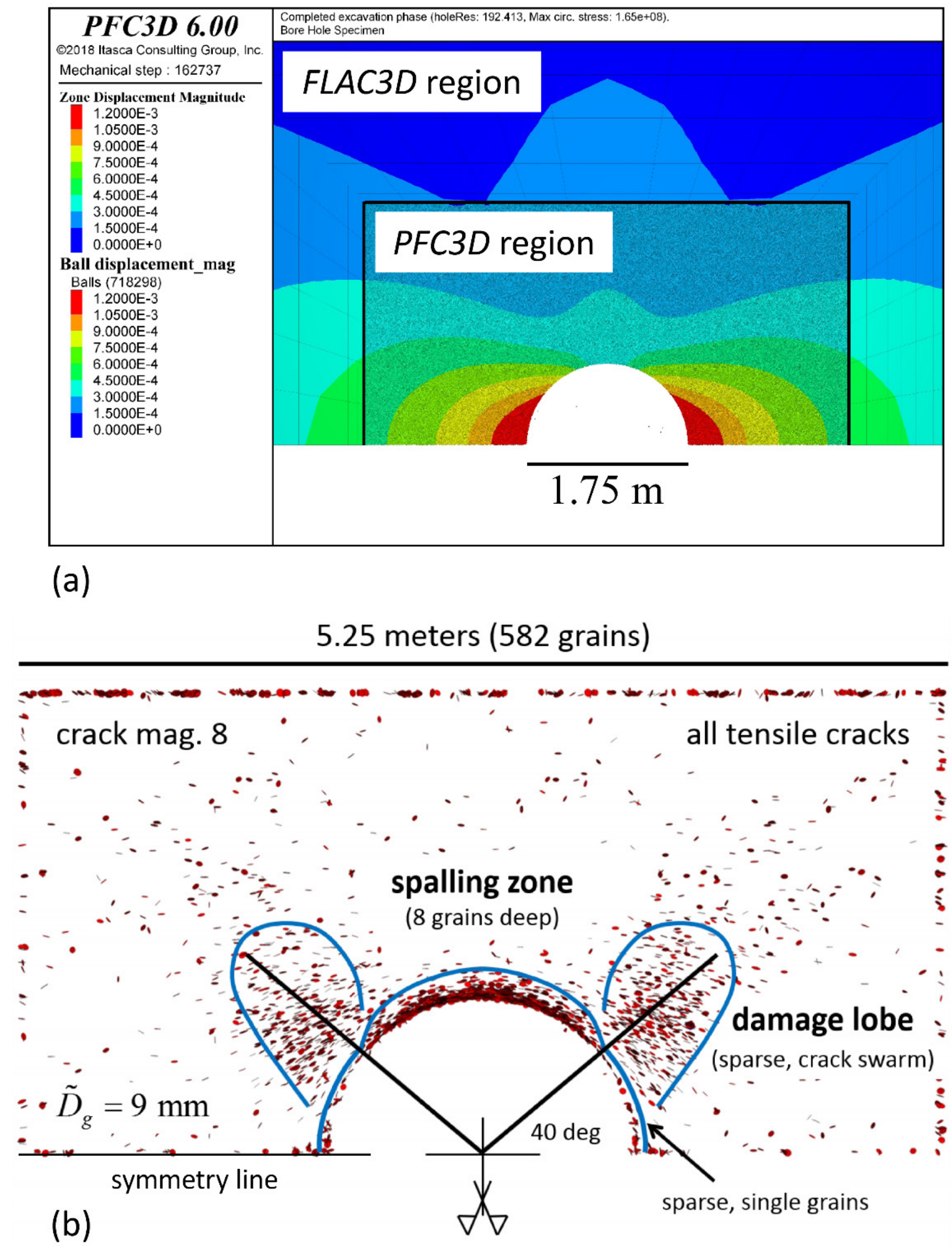

Figure 2. (a) Excavation-induced displacement of the coupled model with 9-mm grain size showing displacement-magnitude contours of the balls and zones. (b) Damage summary overlaid on damage after excavation. The crack magnification is chosen to draw each crack as a disk with a 36-mm diameter. When the cracks are magnified in this way, the crack density cannot be visually assessed, appearing larger than it is because the neighboring cracks overlap one another.

Damage consists of a spalling zone and two damage lobes. The spalling depth is 8 grains over a 100-degree sector and reduces to sparse single grains over the remaining perimeter. The damage lobes consist of a crack swarm located at 40 degrees from the horizontal and extending by the distance of the hole radius into the rock. The crack density and dilation are greater in the spalling zone than in the damage lobes, and the swarm cracks are aligned with the compressive force chains. The spalling zone corresponds with an early stage of rock mass yielding before a well-defined v-shaped notch has formed. The cracks in the spalling zone are like the rock chips that formed in the APSE experiment: formed in tension, aligned parallel to the surface, and dilated. Discrete chips have not formed in the model; such chips might form if the model grain size was reduced to equal the grain size of Äspö diorite. It is likely that the damage lobes are formed where the stress is near to or greater than the crack-initiation stress. The crack-initiation stress of the model material is less than that of the rock (60 versus 90 MPa, respectively); thus, these lobes may be present only in the model and not in the APSE experiment. They were not detected by the AE monitoring of the experiment; however, damage in the lobe regions may be occurring as individual (not clustered) grain-scale cracks that have not been detected by conventional acoustic emission monitoring. The damage lobes are also present in a 2D borehole model of the APSE experiment; however, the damage lobes are not well formed until the APSE load has been scaled up by a factor of two.

Two variants of the base material that match the Äspö diorite properties listed above were created and used in the borehole modeling. In the first material, 25% of the fully bonded interfaces were replaced with slits to increase the Poisson's ratio. In the second material, a distribution of microstrengths was used. The overall damage characteristics (spalling zone and two damage lobes) were only minimally affected by these material modifications.

4 CONCLUSIONS

The *PFC3D* flat-jointed material can be used to model spalling. By using a coupled *FLAC3D*-*PFC3D* model, a 9-mm grain size for a model that approximates the 1.75 meter diameter APSE experiment could be run in a reasonable amount of time (48 hours). This model produced a spalling zone and two damage lobes. The spalling zone corresponds with an early stage of rock mass yielding before a notch has formed with tensile cracks aligned parallel to the hole surface and dilated. Work is planned to model the URL Mine-by Experiment (Martin 1997) using *PFC3D* flat-jointed, soft-bonded and bonded-block models to provide a quantitative assessment of *PFC3D* spall-modeling capability.

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