Technical Memorandum

Date: September 28, 2016

To: PFC development files

From: Jason Furtney

Re: *PFC3D* modeling of rock fragmentation by pressure pulse.

Ref: 8528-03

PFC3D is used to investigate the response of rock blocks to chemically induced pressure pulses. Numerical experiments are conducted on 25 cm cubes of rock with 3.8 cm diameter cylindrical cavities (holes). The holes extend the length of the cube or are limited to the middle 7.8 cm of the cube. The cavities are filled with a chemical mixture in which the reaction is initiated. The pressure resulting from the reaction fragments the rock block.

Itasca's discrete element software *PFC3D* is used to represent the rock and model the fracturing process. The Itasca material-modeling support package (Potyondy, 2016) is used to create specimens of spherical-grain parallel-bonded synthetic material, which are subject to explosive loading. Three specimens are created, a coarse-grained 25 by 25 by 10 cm box, a fine-grained 25 by 25 by 10 cm box, and a coarse-grained 25 cm cube. The coarse models have an average particle diameter of 8.5 mm and the fine model has an average particle diameter of 4.25 mm. The coarse model particle diameters were chosen to result in a specimen with approximately 10,000 particles.

Each specimen consists of a packing of spherical particles connected by parallel bonds. Table 1 gives the material microproperties. The essential micro properties are density (1960 kg/m3), modulus (1.5e9 Pa), normal to shear stiffness ratio (1.5), cohesion (20e6 Pa) and tensile strength (1e6 Pa). A full description of all the microproperties in Table 1 is given in (Potyondy, 2016). These microproperties give rise to the following macroscopic properties: a Young's modulus of 1.82e9 Pa, a (static) direct tensile strength of 0.74e6 Pa and an unconfined compressive strength of 3.4e6 Pa. The material specimens are created without a hole. The material specimens are initially under zero stress.

Table 1 Microproperties of Parallel Bonded Material

Property	Value
Common group:	
N_m	SS_ParallelBonded
$T_m,\ \alpha,\ C_\rho,\ \rho_v\ [\mathrm{kg/m^3}]$	2, 0.7, 1, 1960
$S_g,\ T_{SD},\ \{D_{\{l,u\}}\ [\mathrm{mm}],\ \phi\},\ D_{mult}$	0, 0, {8.0,9.0,1.0}, 1.0
Packing group:	
$S_{RN},\ P_m\ [\mathrm{kPa}],\ \varepsilon_P,\ \varepsilon_{\lim},\ n_{\lim}$ $C_p,\ n_c$	$10000,\ 100,\ 1\times10^{-2},\ 8\times10^{-3},\ 2\times10^{6}$ 1, 0.35
Parallel-bonded material group:	
Linear group:	
$E^*\ [\mathrm{GPa}],\ \kappa^*,\ \mu$	1.5, 1.5, 0.4
Parallel-bond group:	
$g_i\ [\mathrm{mm}],\ \bar{\lambda},\ \bar{E}^*\ [\mathrm{GPa}],\ \bar{\kappa}^*,\ \bar{\beta}$	0.5, 1.0, 1.5, 1.5, 1.0
$(\bar{\sigma}_c)_{\{\mathrm{m,\ sd}\}}\ [\mathrm{MPa}],\ (\bar{c})_{\{\mathrm{m,\ sd}\}}\ [\mathrm{MPa}],\ \bar{\phi}\ [\mathrm{degrees}]$	{1.0,0}, {20.0,0}, 0
Linear material group:	
$E_n^*\ [\mathrm{GPa}],\ \kappa_n^*,\ \mu_n$	1.5, 1.5, 0.4

For this type of loading the tensile strength is expected to be the most important parameter. Additional work can be performed for more complete material properties calibration using flat jointed material, which would allow matching both the UCS and tensile strength.

Physically, the pressure in the hole is controlled by several interactive processes including the chemical reaction, the product equation of state, the deformation of the rock, and the gas flow into the newly created fractures. The goal of this modeling effort is to examine the mechanical response of rock due to loading from a pressure pulse. As a simplification, the pressure in the hole is assumed to follow a predefined path. As a modeling simplification the pressure is assumed to be the same everywhere in the hole at a given time. Pressure is defined as a piece-wise function of time. An initial region of linear increase to a given peak pressure occurs over a given rise time followed by a region of exponential decay.

$$p(t) = \begin{cases} \dfrac{p_p t}{t_r} & when\, t < t_r \\ p_p e^{\lambda(t-t_r)} & else \end{cases}$$

$$\lambda = \ln\left(\frac{1}{2}\right)/t_d$$

Where p_p is peak pressure, t_r is rise-time, and t_d is the time for the pressure to drop to half of the peak value (t_d is taken as five times the characteristic time, discussed below). Figure 1 shows the applied pressure p as a function of time *t*.

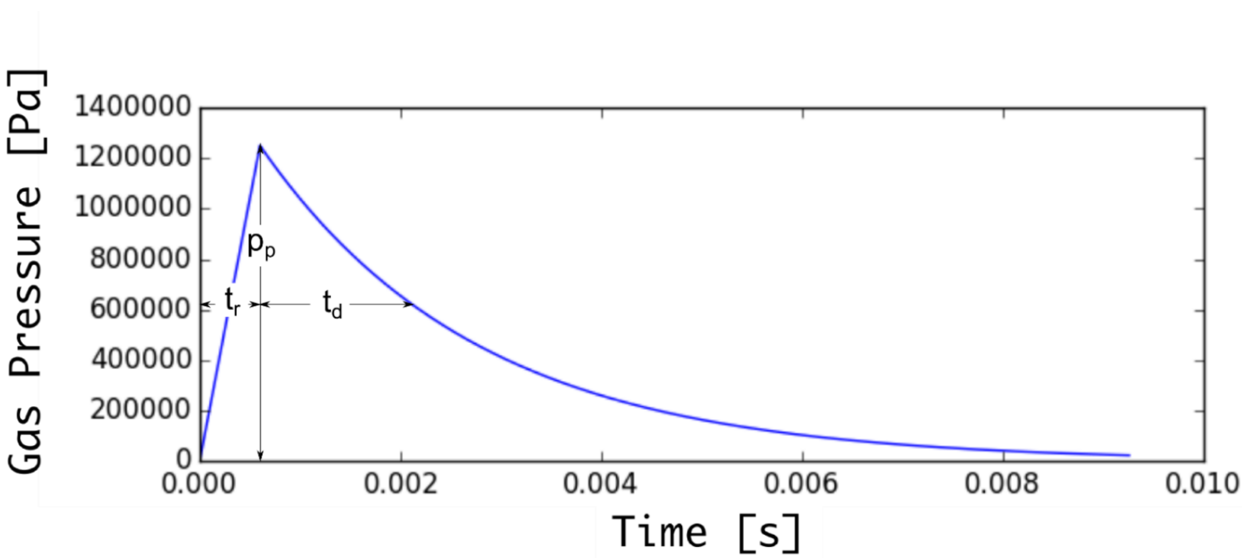

Figure 1 Predefined pressure pulse used in this study.

1.1 Parameter Study on Coarse 25 by 25 by 10 cm Model

A parameter study is conducted to show the effect peak pressure and rise time have on the block fragmentation. A 3.8 cm diameter hole is created, parallel to the *z*-axis, along the entire length of the specimen by deleting the *PFC3D* particles in this region. Particles bordering the inside of this hole are tagged for pressure application. A force equal to pressure divided by particle diameter squared is applied to these tagged particles in the radial direction away from the hole centerline. The tagged particles are used as the pressure application site throughout the model run. As the position of the tagged particles changes, the local radial direction used for pressure application is recalculated.

The peak pressure and the rise time are varied in a 5 by 5 matrix of model runs. Dimensionless quantities for peak pressure and rise time are introduced. The peak pressure is scaled by a characteristic pressure, p_c, taken as the micro tensile strength (1e6 Pa). Rise time is scaled by a characteristic time, t_c, taken as the time required for a p-wave to travel the specimen length. A one dimensional estimate of the sound speed *c* is used, $c = \sqrt{modulus/density}$ = 875 m/s. The length of the specimen is 25 cm, which gives a characteristic time, t_c, of 2.9e-4 s.

A matrix of 25 models is run with peak pressures of 0.75, 1.0, 1.25, 1.5, and 2.0 times p_c and rise times of 0.1, 0.5, 1, 2, and 10 times t_c. Figure 2 shows cross-sections of the middle 2 cm of the 25 *PFC3D* models; the view is down the *z*-axis along the hole. Parallel bond breaks for each of the 25 cases in the parameter study are shown. Black dots represent bond breaks that separate two fragments. Red dots represent bond breaks that are internal to a fragment. Fragments are defined as groups of *PFC* particles that are connected via intact parallel bonds. The fragment plots in Figure 3 are composed of concave triangular surface meshes of the individual fragments. A three-step process generates the surface meshes. (1) A Delaunay tetrahedralization of the centroids of all the particles in a fragment is found. (2) Triangular faces are removed if they have an edge length greater than four times the average particle radii. (3) Triangular faces on the interior of the model are removed. The resulting surface mesh connects the centroids of particles on the exterior of a fragment.

The results of this work show the variation in fracturing with changes in dimensionless rise time and dimensionless peak-pressure. Additional model runs with a range of dimensional parameters could determine the range of values over which this dimensionless scaling would be applicable.

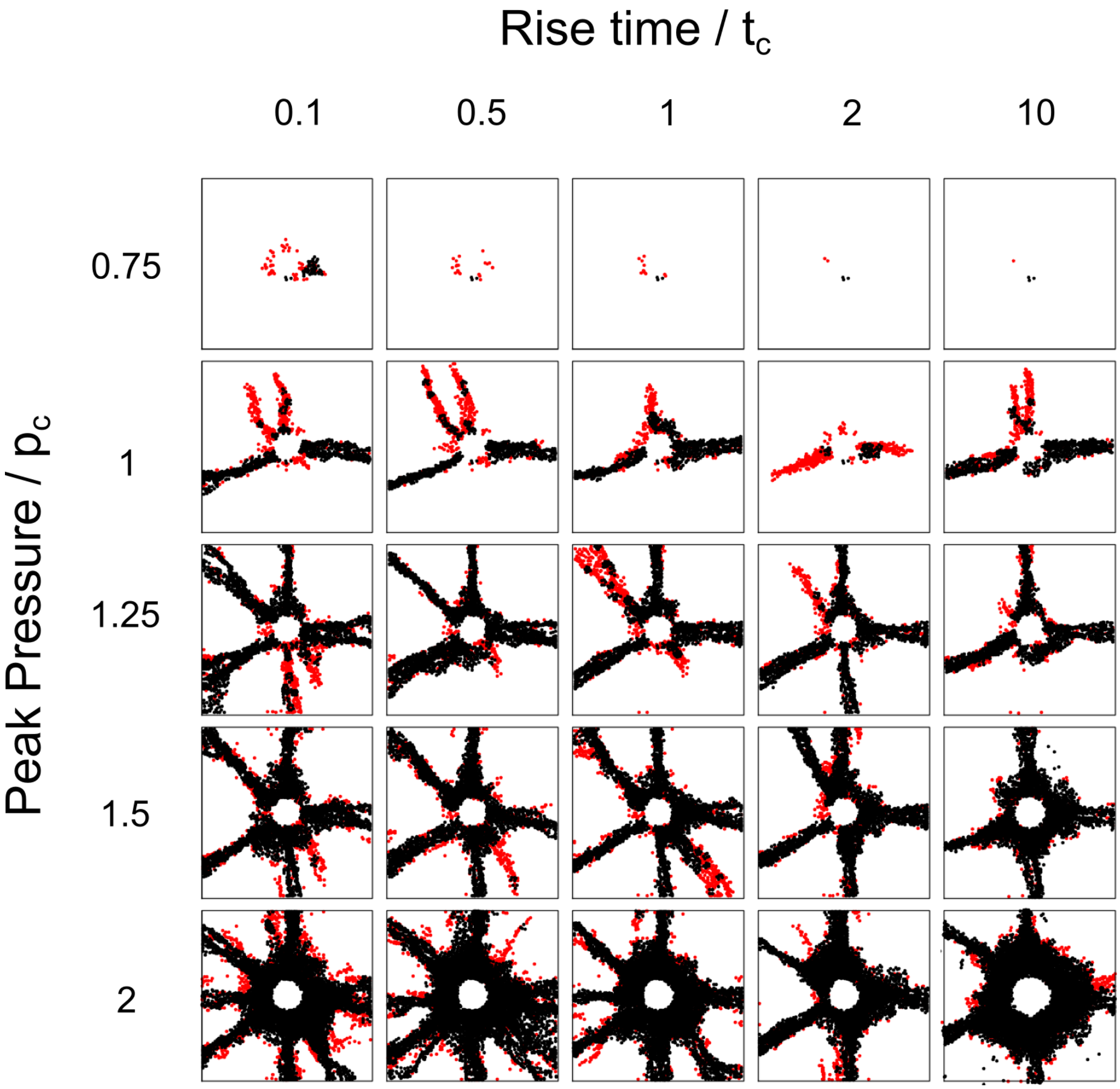

Figure 2 Bond breaks predicted for the 25 cases in the parameter study.

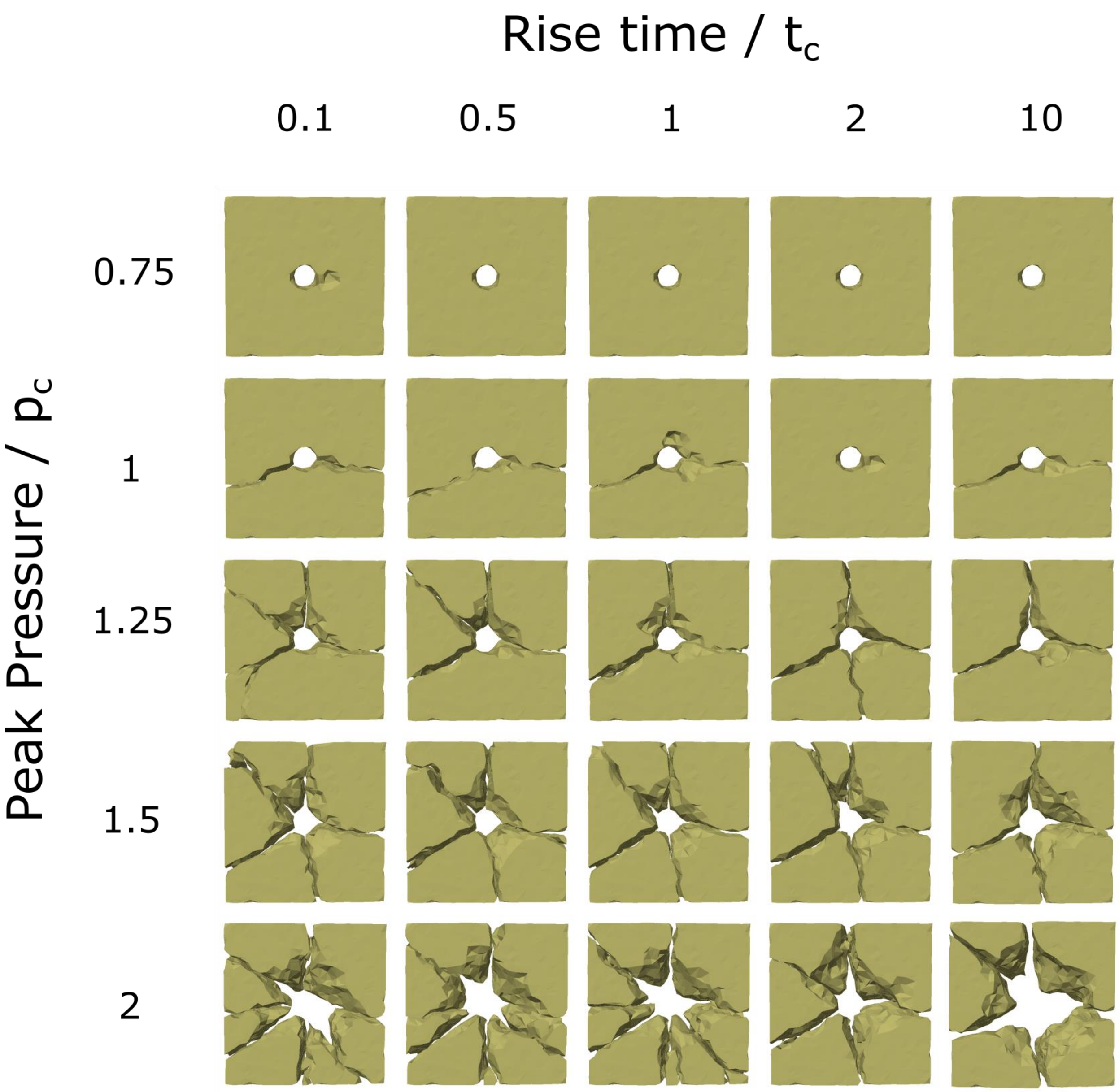

Figure 3 Block fragments created in the 25 cases in the parameter study.

Figure 3 shows the fragments created in each of the 25 cases. The following conclusions are drawn from this study:

- Peak pressures below p_c result in few bond breaks.
- Peak pressures above 1.5 p_c result in a region of intense bond breaking adjacent to the hole.
- Faster pressure rise times give a larger number of discrete radial fractures.

The case with rise time of 2 t_c and peak pressure of 1.25 p_c is considered the base case. This base case is used in the next two sections to investigate the role of model resolution and three-dimensional geometries. Figure 4 shows the pressure and the total number of bond breaks as a function of time for this base case. The number of bond breaks increases quickly for a period of time near the peak pressure. Bond breaking continues at a lower rate after the peak pressure. 90% of the bond breaks occur by 5 ms after the peak pressure.

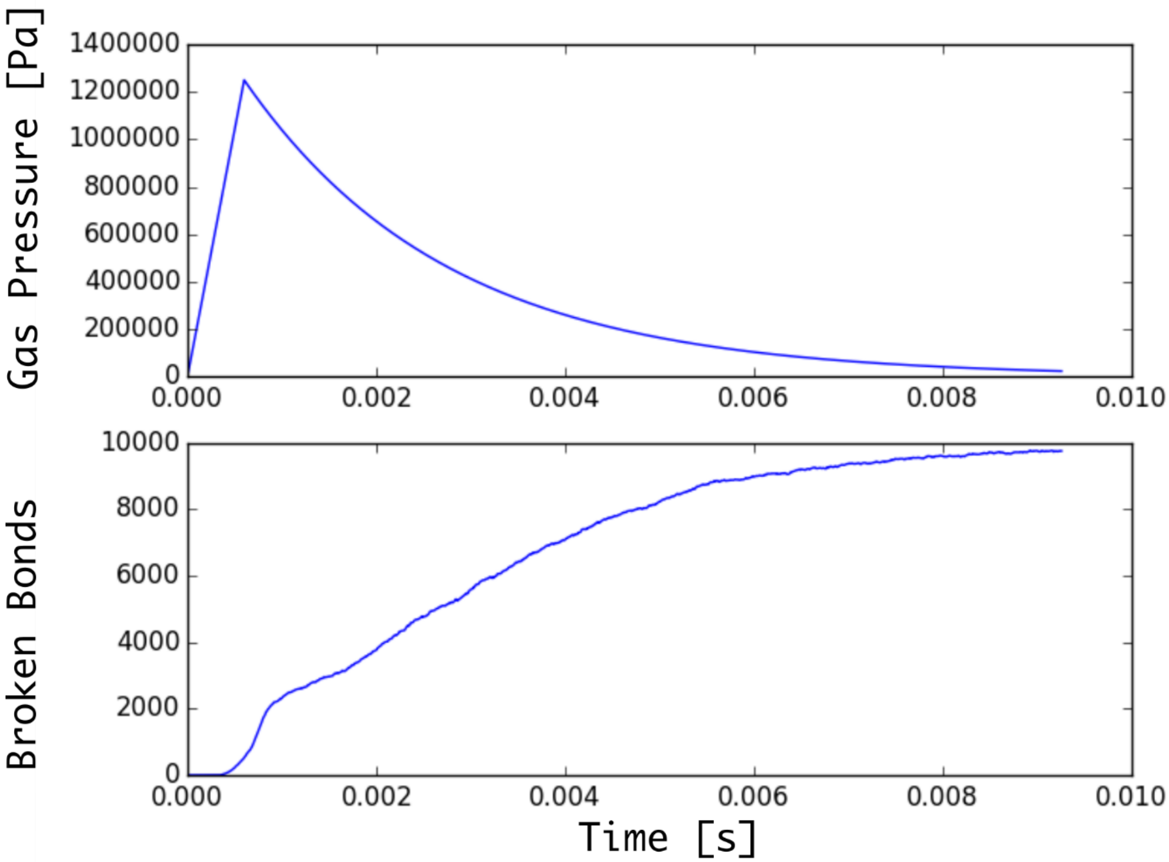

Figure 4 Pressure and bond breaks shown as a function of time for the base case.

The modeling in this work focuses on the damage processes occurring during and shortly after this sharp pressure increase. The duration of the model runs is 10 ms during which most of the fragmentation occurs. If the pressure increase occurs over a period of seconds or minutes, the physical processes occurring would be closer to hydraulic fracturing by its nature. Modeling of hydraulic fracturing requires a different methodology, which incorporates fracture flow and leak-off, is needed. Additional information about the peak pressure and rise times coming from an investigation of the chemical kinetics could help in clarifying the nature of the processes.

In this modeling, the synthetic rock specimen is under zero stress at the beginning of the model runs. If the material is confined, a greater gas pressure would be needed to cause fracturing and damage.

1.2 Model Resolution Effects

The base case from the previous section (rise time of 2 t_c and peak pressure of 1.25 p_c) is used to investigate the effect of particle size on the model result. A specimen with the same 25 cm by 25 cm by 10 cm shape is created with half the particle diameter. The finer specimen has around 100,000 particles. The material properties, hole diameter, and loading procedure are the same as the parameter study described above. Figure 5 provides a comparison between the fragments created in the coarser and fine base cases. The finer case, shown on the right, has five radial fractures with two groups of two closely spaced radial fractures. The coarse base case shown on the left has four approximately equally spaced radial fractures. Although the fine and coarse models have some qualitative similarities, more investigation is required to understand the effect of particle resolution on fracturing.

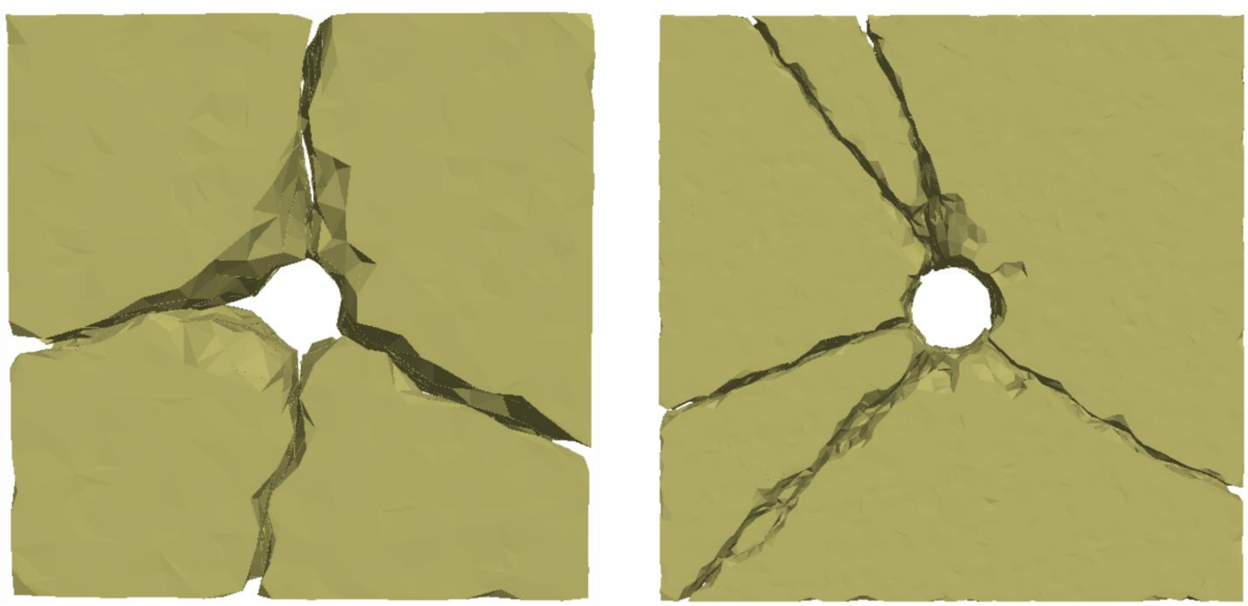

Figure 5 Comparison between fragmentation in the coarse model (left) and fine model (right).

It was expected by Itasca that the finer model would show a proportionally larger number of bond breaks because the effective mode 1 fracture toughness of the finer model is lower. The fracture toughness of bonded particle models is discussed by Potyondy and Cundall (2004). This paper shows that mode 1 fracture toughness is proportional to square-root of particle radius, and so it is expected that the toughness of the fine material is less than that of the coarse material by a factor of $1/\sqrt{2}$. For the case of halving the particle diameter, this scaling does not have a strong effect. For larger changes in particle size this scaling may need to be applied to have material specimens with a constant fracture toughness.

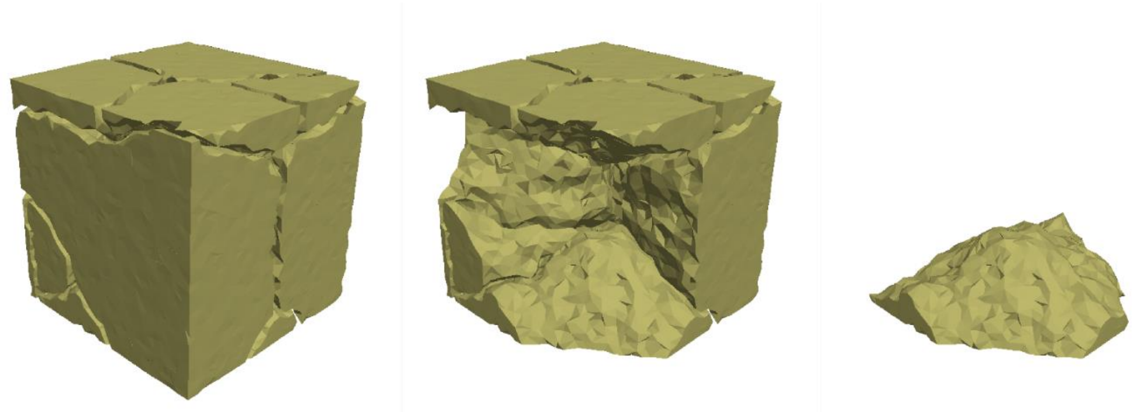

Figure 6 Fragments created in the 25 cm cube model with the hole in the middle of the model only.

1.3 Three-Dimensional Effects

The two previous sections consider a three-dimensional model subject to simplified loading conditions. In these models, the hole extends the length of the specimen and the applied forces are limited to acting in the *x*-*y* plane. This section considers a 25 cm cube specimen with a 7.8 cm long, 3.8 cm diameter hole. The hole is located in the center of the specimen and is aligned along the *z*-axis. The three-dimensional model has around 31,000 particles. The rise time and material properties are the same as in the base case described above. The pressure loading is the same and in addition the gas applies a force upward and downward at the top and bottom of the hole.

Figure 6 shows the fragments created in this case. Three images are shown, with the the leftmost showing all the fragments, the middle showing the fragment nearest the observer removed, and the rightmost showing only the lower fragment. Radial fractures occur around the hole circumference and cone-shaped cracks occur above and below the hole. Similar patterns of fracturing are observed in rock blasting.

A peak pressure of 2.5 p_c is used in this case relative to the 1.25 p_c in the base case. In this case, the hole is limited to the central 7.8 cm of the specimen. A greater peak pressure is needed to create qualitatively similar fractures to the base case for two reasons. First, both radial and cone fractures are created resulting in greater fracture surface area. Second, these fractures are created by proportionally less reaction products. The surface area over which the pressure pulse is applied is smaller which results in less mechanical work done by the gas on the rock.

1.4 Data Files

A set of Python programs perform these model runs. Python is a programming environment which is embedded in *PFC3D*. Using Python with *PFC3D* is described in the *PFC3D* manual and in Furtney et al., (2016). Running the file master.p3dat runs all the models described in this report. The file README.txt gives more description of the individual files. The data files in the folder "coarse_box/" are used to generate the coarse specimen for this parameter study. Running "myMatGen.p3dvr" creates a model state file, which is used as the starting point of this parameter study. The file "load.py" defines the hole excavation and pressure loading. The file "parameter_study.py" runs the 25 case parameter study. The folder "fine_box/" contains the files that create the fine specimen, and the folder "cube/" contains the files for the dimensional specimen. The files "base_fine.py" and "base3d.py" run the fine model and 3D model.

REFERENCES

Furtney, J.K., M. Purvance and S. Emam. (2016) "Using the Python Programming Language with Itasca Software", **In Proceedings, The Fourth Itasca Symposium on Applied Numerical Modeling, (Lima, Peru, March, 2016)**. Minneapolis, Itasca International, Inc.

Potyondy, D. O., and P. A. Cundall. (2004) "A Bonded-Particle Model for Rock," *Int. J. Rock Mech. & Min. Sci.*, ***41***(8), 1329–1364.

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