

# **An Innovative 3-D Numerical Modelling Procedure for Simulating Repository-Scale Excavations in Rock – SAFETI**

R. P. Young, D. Collins, J. Hazzard, A. Heath  
University of Liverpool, Department of Earth Sciences, UK

W. Pettitt, C. Baker  
Applied Seismology Consultants Ltd., UK

D. Billiaux, P. Cundall, D. Potyondy, F. Dedecker  
Itasca Consultants S.A., France

C. Svemar  
SKB, Sweden

P. Lebon  
ANDRA, France

5 page manuscript submitted to Euradwaste '04 Conference, Luxembourg, March 29-31 2004

## **Summary**

This paper presents current results from work performed within the European Commission project SAFETI. The main objective of SAFETI is to develop and test an innovative 3D numerical modelling procedure that will enable the 3-D simulation of nuclear waste repositories in rock. The modelling code is called AC/DC (Adaptive Continuum/DisContinuum) and is partially based on Itasca Consulting Group's Particle Flow Code (PFC). Results are presented from the laboratory validation study where algorithms and procedures have been developed and tested to allow accurate 'Models for Rock' to be produced. Preliminary results are also presented on the use of AC/DC with parallel processors and adaptive logic. During the final year of the project a detailed model of the Prototype Repository Experiment at SKB's Hard Rock Laboratory will be produced using up to 128 processors on the parallel super computing facility at Liverpool University.

## **1. Introduction**

The combination of numerical modelling and observational validation has led to significant recent advances in our understanding of the evolution of the Excavation Disturbed Zone. However, most applications of numerical modelling to repository excavation problems are restricted in that they either (i) involve rather simplistic models that do not account for the detailed response of the rock with time or (ii) consider more complex models but are restricted to small scales and/or 2-D cases. The SAFETI project is developing a highly innovative code that will allow a more 'realistic' simulation of repository excavations in 3-D to be carried out.

## **2. Methodology**

The discrete element (discontinuum) portion of the AC/DC code is based on the PFC3D code developed by the Itasca Consulting Group. The code works by initially considering the rock mass as a continuum. As 'elements' of the rock-mass respond to stress from excavation disturbance (or other influences) these convert to a discontinuum response in order to track the development of cracking as it occurs. The code has been developed to run on the multiple-node parallel super-

computing facility (NESSC) at Liverpool University. This allows significantly larger-scale simulations to be run than have been possible to date.

### 3. Results

The AC/DC codes are undergoing calibration and validation as part of the SAFETI project. The first phase has involved a comprehensive set of laboratory true-triaxial tests where mechanical, velocity and acoustic emission (AE) data have been collected and simulated. The second phase of the project is concerned with comparing numerical simulations and actual in-situ velocity and AE data from the Prototype Experiment at SKB's Hard Rock Laboratory (HRL).

#### 3.1 Laboratory Validation Study

Laboratory experiments have been performed at Imperial College London using a true triaxial loading frame. The tests involved loading a 5cm cube sample of Crosland Hill sandstone through a complex loading history designed to determine the response of the sample to both stress effects and damage. The main phases are shown in Figure 1, and involve initial hydrostatic loading and unloading of the undamaged sample, followed by deviatoric loading to induce fractures in the sample, and finally hydrostatic loading and unloading of the damaged sample. During the load history a variety of geotechnical and geophysical data were collected with time. This included recording P-, S1-, and S2-waveforms in each of the 3 principle directions, allowing dynamic moduli values to be determined. At the same time, a stress probe measurement in each principle direction was performed to allow the calculation of static moduli values in the sample. Additionally 24 sensors were used to record acoustic emission (AE) waveform data during the test. Figure 2 presents the 9142 AE events that were located. Clusters of events are observed to propagate across the sample in time. The events appear to delineate a series of macroscopic fractures across the sample that are oriented semi-parallel to the  $S_1$ - $S_2$  plane.

#### 3.2 Developments in PFC3D Modelling Algorithms and Procedures

A well-defined procedure has been produced to generate a PFC3D material and assign microproperties that can match the short- and long-term behaviour of hard rock. The time-dependent behaviour is modelled using a 3D stress corrosion algorithm. An elastic stiffness probe has been developed to measure static moduli values in all directions. A methodology for dynamic wave propagation in PFC3D models has been formulated, allowing the calculation of dynamic moduli values. A set of functions have also been written and tested to record AE in the models and calculate locations, magnitudes and mechanisms. Each bond break is considered a crack, and an AE can be equal to one or more cracks. A method of grouping cracks together that occur in similar space and time has been produced, and this is found to produce realistic AE event numbers and magnitudes.

Figure 3a presents the stress history for the true triaxial laboratory test, showing the two initial hydrostatic loading phases, followed by the deviatoric loading phase, and the final hydrostatic loading phase. Figures 3b and 3c present the measured and modelled velocity results. Both sets of data show similar trends with velocity increase during hydrostatic loading and decrease during unloading. During the deviatoric loading, both the model and actual rock show similar decreases in the velocity of waves propagating in the minimum stress direction. Some quantitative differences in the velocity change values are noticed between the model and rock during hydrostatic loading. This is believed to be due to the PFC3D material not including pre-existing pore space and microcrack structure. This issue is being considered in future models.

### **3.3 Field Scale Study**

The Prototype Repository Test (PRT) at SKB's Hard Rock Laboratory (HRL) has been chosen to be modelled using AC/DC. The PRT has been designed to simulate a disposal tunnel in a real repository for storage of high-level nuclear waste. The main gallery is a 5m diameter sub-horizontal tunnel excavated in a dioritic granite using a tunnel boring machine (TBM). Six full-scale 1.75m diameter deposition holes have been excavated vertically to 8.8 m using a smaller TBM. AE and velocity survey data were collected during the excavation of two of these holes. Figure 4 shows the AE locations around one of the holes, and the insert diagram shows examples of straight raypaths between pulsing and receiving sensors from the velocity surveys.

### **3.4 Development and Testing of the AC/DC Code**

The AC/DC code has been written allow 3D adaptive models to be generated and run on multiple processors. The base code uses a periodic cell (PBRICK) concept to allow large models to be quickly built up, as well as allowing the model to be easily divided between parallelised processors. Each PBRICK can be represented as either a particle or matrix brick. Particle bricks are based on a densely packed assembly of PFC3D particles. The matrix brick is a more simple representation which does not have particles and can not therefore break apart. This is a reasonable assumption in regions where microcracking is not expected, and also makes the model much more computationally efficient. Adaptive logic has been written to convert matrix PBRICKS to particle PBRICKS as required near regions of new bond-breakages (microcracking). Figure 5 presents two time steps from an AC/DC model made of 36 PBRICKS. Following the creation of new microcracks the model is seen to convert a number of the matrix PBRICKS into particle PBRICKS. Results from AC/DC are viewed using a custom developed 3D visualization program called ACDCVIS.

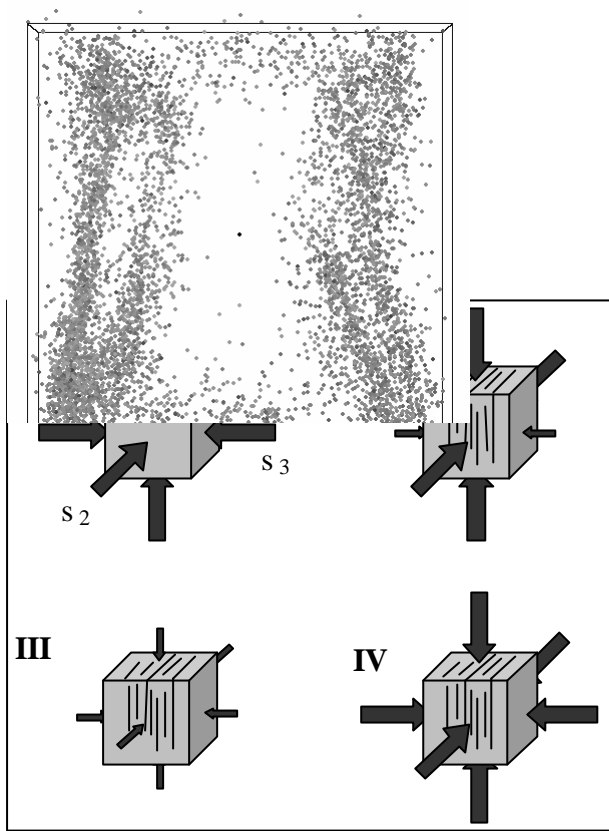
Initial testing of the AC/DC code on the super computer at Liverpool University has been performed. Models were produced entirely of particles and others a combination of particle and matrix PBRICKS. Models were run on one processor and also split between 6 processors. By using a combination of matrix and particle PBRICKS and by intelligently dividing up a model over six processors compared to one, a model can be run in less than 10% of the time required by a traditional PFC model. This is expected to reduce by a further order of magnitude when 10's of processors are used in parallel to run the model.

## **4 Discussion and Conclusions**

An innovative new modelling code termed AC/DC has been written to produce realistic 3-D simulations of field scale repository tests. The code uses periodic cells and adaptive logic allowing it to run on multi-processor supercomputers. The code has currently been successfully tested in parallel on 6 processors and it is planned to use over 100 processors on the super computer at Liverpool University for the field scale model.

A set of laboratory true triaxial loading tests have been performed to produce data sets of static and dynamic moduli and AE activity in a rock sample during hydrostatic and deviatoric loading. This data has allowed procedures and algorithms to be developed to produce accurate 'Models for Rock'.

It is expected that the AC/DC methodology will become a standard and basis for future simulations of nuclear waste repositories at excavation scale.



## 5 Acknowledgements

This Project is co-funded by the European Commission and performed as part of the fifth EURATOM framework programme, Nuclear Fission (1998-2002 ).

Figure 1: A schematic diagram presenting the main phases in the true triaxial laboratory test with the thick and thin arrows representing high and low acting stresses. The test involved hydrostatic loading and unloading of the undamaged sample, deviatoric loading of the sample leading to fracture creation, and hydrostatic loading of the damaged sample.

Figure 2: The locations of the acoustic emissions recorded during the true triaxial test. The view is looking in the  $\sigma_2$  direction, and the results suggest a number of subvertical fracture surfaces have formed.

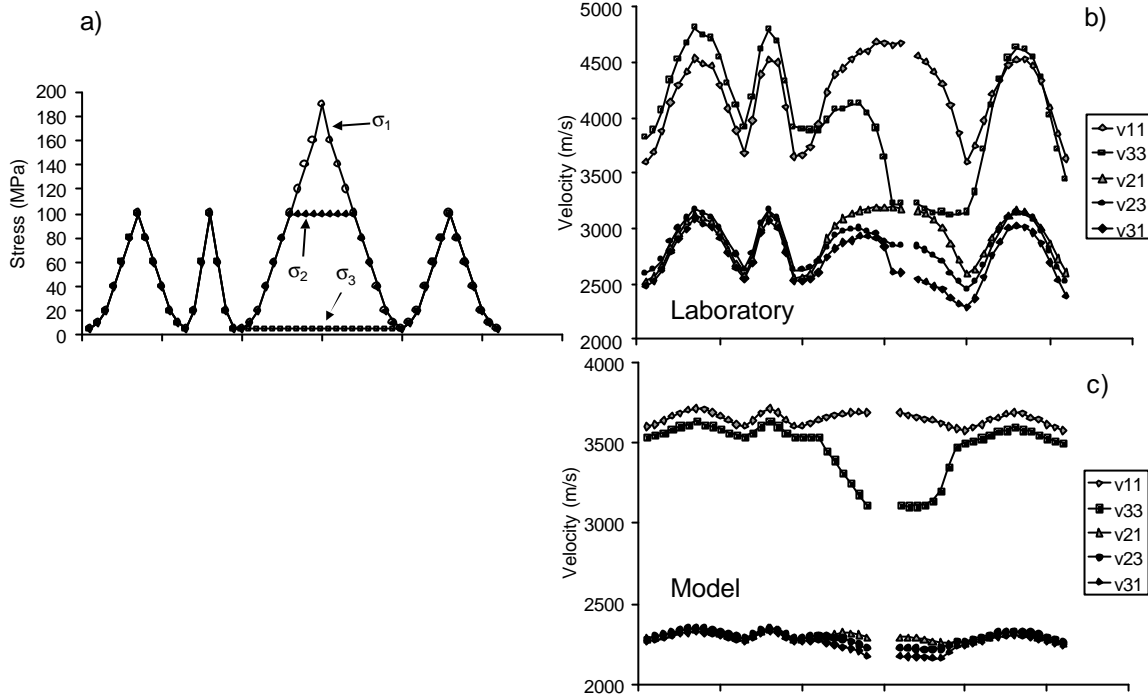


Figure 3: a) Maximum, intermediate and minimum principal stresses applied to the laboratory sample and model ( $\sigma_1$ ,  $\sigma_2$  and  $\sigma_3$  respectively), b) measured velocities in the laboratory experiment (some components are omitted for clarity). The two subscripts refer to the propagation direction and polarization direction respectively. The numbers 1, 2 and 3 correspond to the directions of  $\sigma_1$ ,  $\sigma_2$  and  $\sigma_3$ , c) Velocities in the model.

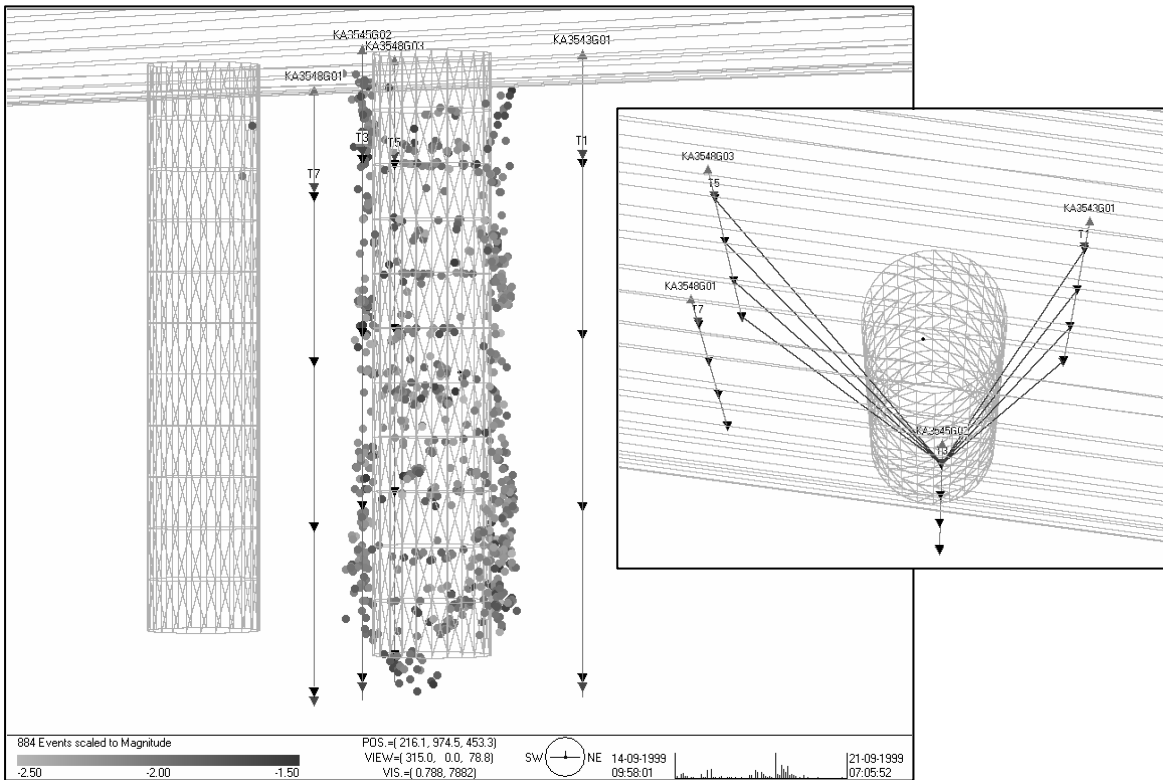


Figure 4: The Prototype Repository Test at SKB's Hard Rock Laboratory has been chosen for the field scale modelling study. Locations of acoustic emissions during the canister hole excavation are shown. The insert diagram displays some of the raypaths where repeat velocity surveys have been performed.

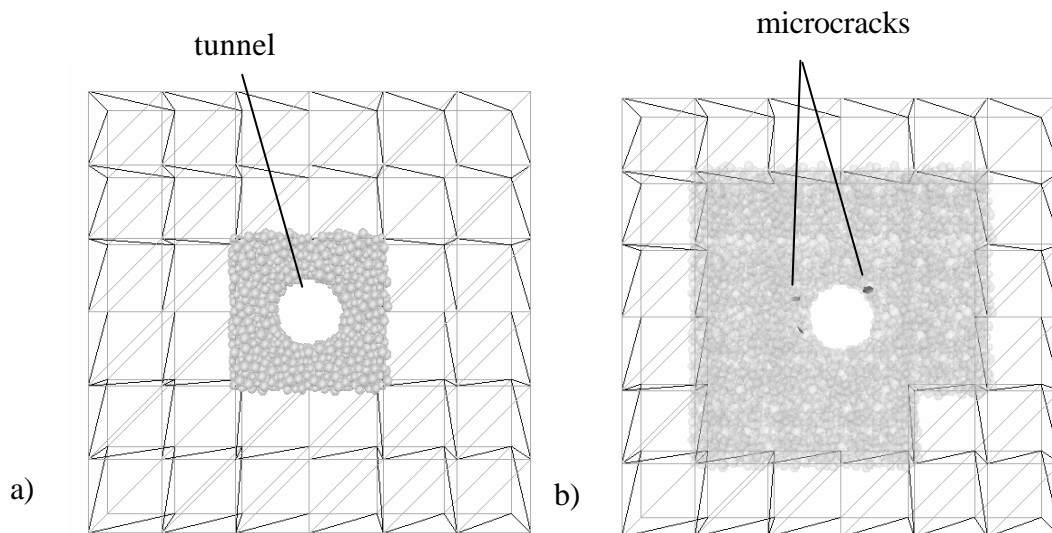


Figure 5: a) An AC/DC model made of a combination of 32 full-matrix PBRICKS (periodic cells) and 4 particle PBRICKS. A tunnel has been created in the center of the sample. b) The same AC/DC model following the creation of stress induced bond-breakages interpreted to be microcracking. The adaptive logic incorporated into the AC/DC model has converted a number of the full-matrix bricks into particle bricks near the regions of microcracking.