1 Abstract

Discrete Element Methods (DEM) explicitly model the mechanics of the discontinuities of naturally fractured rock masses. However, due to the large number of degrees of freedom in DEM simulations and the requirement of small times steps, the application of DEM simulations to reservoir-scale problems and long-term fluid injection problems is often computationally prohibitive.

In order to reduce the computational costs associated with full-scale DEM simulations, an up-scaling method is presented in which Representative Elementary Volume (REV) DEM simulations are used to calibrate the parameters of a Continuum Damage Mechanics (CDM) constitutive model that is then used for Finite Element Analysis (FEA). The CDM model empirically captures the effect of the degradation of the rock integrity due to the yielding and sliding of natural fractures in the rock mass.

Up-scaling is achieved through homogenization, in which the spatially averaged stress-strain behavior of various DEM RVE simulations is computed. Subsequently, a CDM constitutive relationship is fitted using the Levenberg-Marquardt Algorithm (LMA) and the homogenized DEM simulation data. The CDM model is then used in FEA reservoir scale simulations. The CDM model is implemented in ABAQUS$^{\text{TM}}$ and DEM simulations were conducted using UDEC$^{\text{TM}}$. The up-scaling methodology is demonstrated through a case study on a naturally fractured carbonate reservoir in which the up-scaled CDM model compares well with a direct numerical simulation with the DEM model but requires an order of magnitude less computational time.

2 Introduction

Discrete Element Method (DEM) models are used commonly in geomechanics to explicitly model the mechanics of Naturally Fractured Rock (NFR) masses (Jing, 2003). NFR is often modeled as a multiscale material due to the vastly different length scales involved in the deformation process (Zhou et al., 2003). At the fracture scale (10-3 m), the physics is dominated by brittle fracture propagation and fracture-to-fracture contact force interaction, while one is normally interested in the reservoir scale (103 m) response as a result of the spatial extension of the fractures. Because these scales of interest span approximately six orders of magnitude, multiscale methods are required to assess the overall response as modelling with fracture scale resolution at the reservoir scale becomes computationally prohibitive.

DEM models, unlike standard continuum models, consider the fractures within the rock mass as a Discrete Fracture Network (DFN), which explicitly defines the geometry of the fracture network. The physics of block interaction is then governed by the motion, contact forces and traction-separation laws between the rock blocks and the fractures (Cundall and Strack, 1979). Because NFR behavior is complex, even sophisticated phenomenological constitutive relationships may be inadequate to describe the complete rock mass behavior.

The DEM approach aims to address this continuum behavioral deficiency by only requiring constitutive relations for the block interactions. (Cundall, 2001).

That being said, the main issue with DEM models is primarily the computational demands. Due to the large number of degrees of freedom in the models and the requirement for very small time steps because of the constant need for contact detection between blocks running reservoir scale models is computationally prohibitive. The intent of this article is to develop a framework that incorporates the response of the DEM models while harnessing the computational speed of the continuum models. Up-scaling is accomplished in this paper by calibrating a continuum model with DEM virtual experimental data using an iterative least squares regression algorithm.

The general goal of up-scaling is to formulate simplified coarse-scale governing equations that approximate the fine-scale behavior of a material (Geers et al., 2010). In the case of the DEM simulations in this investigation, the aim of up-scaling is to identify the parameters of a continuum model that best mimics the response of the DEM model.

Multiscale methods that can be considered often fall into one of two classes: hierarchical or concurrent (Gracie and Belytschko, 2011). In concurrent multiscale models, different scales are used in different regions of the domain; the solution of the coupled model proceeds by solving both scales simultaneously. This approach is very expensive since the time step of the whole simulation is controlled by the fine-scale model; however, the solution is often more accurate. In hierarchical multiscale methods, the constitutive behavior at the coarser scale is determined by exercising a finer scale RVE. The finer scale models vary from relatively simple models, as in micromechanics, to complex nonlinear models. This approach is much more efficient, but can be less accurate. Up-scaling in this investigation can be considered to be a hierarchical multiscale method using computational homogenization.

Many multiscale homogenization techniques have been developed and proposed in the past, (Aanonsen and Eydinov, 2006; Temizer and Wriggers, 2007; Loehnert and Wriggers, 2005), but none have addressed the problem of upscaling DEM simulations of NFR to continuum damage mechanics models using parameter estimation techniques.

3 Up-Scaling Methodology

The upscaling methodology that is developed in this paper aims to homogenize DEM simulations to estimate a set of parameters in a Continuum Damage Mechanics (CDM) model. In order for this method to be effective, the CDM has to be parameterized by identifying key parameters in the constitutive relationships that govern the behavioral response. The general upscaling methodology presented here can be summarized in three steps:

1. Run REV DEM simulations of NFR under various loading conditions.

2. Apply homogenization algorithms to DEM results to obtain stress-strain curves.

3. Iteratively run a parameterized CDM model within a parameter estimation algorithm to minimize the difference between the CDM and DEM responses.

Once the optimal parameter set for the continuum material model is identified, the newly established constitutive model can be used in a Finite Element Method (FEM) code to simulate the response of NFR at the reservoir scale.

3.1 DEM Simulations

The DEM simulations used in this investigation consist of a DFN within a 10m10m virtual block subject to uniaxial and triaxial testing procedures (Fig 3.1). The nature of numerical modelling allows one the luxury of conducting physically impractical material tests such as direct tensile tests in order to characterize the material properties of the NFR.

Figure 1: Two dimensional DFN used for the DEM simulations. A 10m10m Voronoi tessellation with an average block size of 0.5m was used to characterize the DFN.

The 10m10m model size was determined to be sufficient to represent the DFN, which was characterized by a Voronoi tessellation with a block size of approximately 0.5m. Since the material model used in this investigation can only consider an isotropic NFR, a inherently isotropic randomly generated Voronoi tessellation was chosen to represent the DFN in the DEM simulation. The rock and joint properties for the model, given in Table 3.1, were chosen to be representative of a reservoir rock (Pirayehgar and Dusseault, 2015).

Table 1: Rock and joint properties for the DEM simulations

Property	Value
Rock Density	$2.7kg/m^3$
Rock Young's Modulus	$12GPa$
Rock Poisson's Ratio	0.3
Joint Normal Stiffness	$10GPa$
Joint Shear Stiffness	$1GPa$
Joint Friction Angle	$30°$
Joint Cohesion	$0.1MPa$
Joint Tensile Strength	$10MPa$
Joint Dilation Angle	$10°$

The DEM model was subjected to uniaxial tension and compression cycles as well as triaxial tension and compression cycles under different confining stresses to calibrate the continuum model. The triaxial tests were conducted at confining stresses of 5MPa and 10MPa. These numerical tests were constrained in such a way to imitate the laboratory testing procedures. The only procedural difference in these virtual laboratory tests was that the axial strain is brought back to the initial configuration in order to characterize the damage evolution.

The compression cycles were run at a target strain rate of 0.001/s for a period of 10s in compression followed by a period of 10s in tension to return the strain to zero. The transition from the compression part of the load path to the tension part of the load path was conducted over a period of 2s to avoid shocking the system.

Because the tension cycles reach failure at a much lower strain, the tension cycles were run at a target strain rate of 0.0001/s for a period of 5s in each direction. In this case, the transition period from tension to compression was 1s.

The aim of the compression and tension cycles is to strain the model past the yield stress in order to investigate the post-yield behavior, but not strain the model so much that the RVE loses all of its strength. It is noted that the strain rate was chosen to be sufficiently small so as to avoid strain rate effects. The appropriate amount of strain for a given DEM simulation will depend upon the DEM geometry in addition to the rock and joint properties.

4 Distinct Element Method

5 Homogenization Approach

The main objective of homogenizing DEM simulations is to be able to describe the macroscopic behaviour of the distontinuous medium in term of a standard continuum model. In this homogenization process, the resultant inter-block contact forces and block displacements - resultant from the DEM simulations - are converted to stresses and strains in a continuum mechanical context.

The first logical step in this homogenization procedure is to riggerously define the area of interest to be homogenized. For the homogenization procedure to yeild any meaningful outcome, the homogenization procedure should be applied to a Representative Elementary Volume (REV) for the system. The exact size of the REV functions on the Discrete Fracture Network (DFN) prescribed to the DEM model, and some relavent statistical parameters (insert reference). For this homogenization approach to hold valid, the REV of size d contained within a system with a characteristic length D and consisting of particles with a characteristic diamater δ, must subsribe to the following scale seperation (ref wellman):

$$D \gg d \gg \delta \tag{1}$$

**To avoid indulging on the statistics required to formally define an REV for a particular DFN, an REV is assumed for this purposes of this investigation.

The REV is chosen to be a circular subsection of the DEM model for reasons (in this reference).

Due to the discontinuous nature of the DEM simulations, the circular REV cannot be used dirrectly. Because the calculated displacements and contact forces from the DEM are known at the block edges, the homogenization area boundary must follow the block boundaries. In order to define a homogenization area based on the REV, but subscribing to the block boundaries, the homogenization area is taken to be the area defined by the block boundaries of the blocks that intersect the REV boundary (see figure blah).

************************(figure blah, depicting the homogenization boundary and a close up of the boundary showing the displacment jumps)**************************

One must also note the potential displacement jumps that may occur between blocks on the boundary. In the case where the blocks become physically separated, there exists a discontinuity along the homogenization boundary (again, see figure blah abaove). These discontinuities along the homogenization boundary were considered by adding boundary segments to the homogenization boundary between the corners of the adjacent blocks.

The homogenization boundary, Γ_h, can be described in terms of n ordered boundary vertices, $V_i^h = (x_i^h, y_i^h)$, representing the ith set of vertex coordinates along the boundary, such that the homogenization area, A^h, can be calculated using the following formulation for the area of an arbitrary, non-self-intersecting polygon(find reference):

$$A^h = \frac{1}{2}\sum_{i=1}^{n} x_i^h (y_{i+1}^h - y_{i-1}^h) \tag{2}$$

At this point, within the homogenization area, one must differentiate between the block area and the void area as they have fundamentally different behaviour. The total block area, A^b can be assessed as a summation of m block areas within the homogenization area, while the individual block area can be assessed in a similar manner to 2. For n^j block boundary vertices, $V_{i,j}^b = (x_{i,j}^b, y_{i,j}^b)$ representing the ith set of vertex coordinates on the jth block, the total block area can be calculated as:

$$A^b = \frac{1}{2}\sum_{j=0}^{m}\sum_{i=1}^{n^j} x_{i,j}^b (y_{i+1,j}^b - y_{i-1,j}^b) \tag{3}$$

Assuming that the block area and the void area are jointly exhaustive of the total homogenization area, the total void area, A^v, can be written as the difference of the homogenization area and the block area:

$$A^v = A^h - A^b \tag{4}$$

$$A^v = \frac{1}{2}\sum_{i=1}^{n} x_i^h (y_{i+1}^h - y_{i-1}^h) - \frac{1}{2}\sum_{j=0}^{m}\sum_{i=1}^{n^j} x_{i,j}^b (y_{i+1,j}^b - y_{i-1,j}^b) \tag{5}$$

5.1 Stress Homogenization

Homogenization of the stresses in a DEM simulation generally relies upon the reduction of the inter-particle contact forces to generate an equivalent continuum stress state(ref wellman). However, in UDEC^{TM}, since the blocks are deformable, the contact force reduction is done during simulation time to allow stresses to develop within the block zones. As such, the stress homogenization procedure presented here is formulated around deformable DEM blocks.

For

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{A^h} \int_{\Omega} \boldsymbol{\sigma} dA \tag{6}$$

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{A^h} \left[\int_{\Omega_r} \boldsymbol{\sigma} dA + \int_{\Omega_f} \boldsymbol{\sigma} dA \right] \tag{7}$$

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{A^h} \left[\sum_{i=1}^{N_b} \boldsymbol{\sigma}^i A_b^i + \sum_{i=1}^{N_d} \boldsymbol{\sigma}^i A_d^i \right] \tag{8}$$

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{A^h} \left[\sum_{i=1}^{N_b} \sum_{j=1}^{N_z} \boldsymbol{\sigma}_z^{ij} A_z^{ij} + \sum_{i=1}^{N_d} p_d^i \mathbf{I} A_d^i \right] \tag{9}$$

5.2 Strain Homogenization

$$\boldsymbol{\epsilon} = \frac{1}{2} \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] \tag{10}$$

$$\langle \boldsymbol{\epsilon} \rangle^{\Omega} = \frac{1}{A} \int_{\Omega} \boldsymbol{\epsilon} dA \tag{11}$$

$$\langle \boldsymbol{\epsilon} \rangle^{\Omega} = \frac{1}{A} \left[\int_{\Omega_r} \boldsymbol{\epsilon} dA_r + \int_{\Omega_f} \boldsymbol{\epsilon} dA_f \right] \tag{12}$$

$$\langle \boldsymbol{\epsilon} \rangle^{\Omega} = \frac{1}{2A} \left[\int_{\Omega_r} \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] dA_r + \int_{\Omega_f} \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] dA_f \right] \tag{13}$$

$$\langle \boldsymbol{\epsilon} \rangle^{\Omega} = \frac{1}{2A} \left[\oint_{\Gamma_r} \left[\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u} \right] d\Gamma_r + \oint_{\Gamma_f} \left[\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u} \right] d\Gamma_f \right] \tag{14}$$

$$\langle \boldsymbol{\epsilon} \rangle^{\Omega} = \frac{1}{2A} \left[\sum_{i=1}^{N_{rb}} \left[\mathbf{u}_{rb}^i \otimes \mathbf{n}_{rb}^i + \mathbf{n}_{rb}^i \otimes \mathbf{u}_{rb}^i \right] L_{rb}^i + \sum_{i=1}^{N_{db}} \left[\mathbf{u}_{db}^i \otimes \mathbf{n}_{db}^i + \mathbf{n}_{db}^i \otimes \mathbf{u}_{db}^i \right] L_{db}^i \right] \tag{15}$$

6 Damage Plasticty Model For Quasi-Brittle Materials

Damage plasticity model based on Strain can be decomposed into elastic and plastic components:

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^{el} + \boldsymbol{\epsilon}^{pl} \tag{16}$$

Taking the time derivative gives the decomposition of the strain rate, $\dot{\boldsymbol{\epsilon}}$:

$$\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}^{el} + \dot{\boldsymbol{\epsilon}}^{pl} \tag{17}$$

The constitutive stress-strain relationship including a scalar damage parameter, $\mathbf{D}$ can be written as follows:

$$\boldsymbol{\sigma} = (1 - \mathbf{D})\mathbf{E} : \boldsymbol{\epsilon}^{\boldsymbol{el}} \tag{18}$$

For simplicity, the damaged elastic stiffness is described as the reduced stiffness due to the damage:

$$\mathbf{E^d} = (1 - \mathbf{D})\mathbf{E} \tag{19}$$

Substituting 16 and 19 into 18 results in the following:

$$\boldsymbol{\sigma} = \mathbf{E^d} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{pl}) \tag{20}$$

Using the "usual notions of CDM" (find reference), the effective stress. $\bar{\boldsymbol{\sigma}}$, can be defined as:

$$\bar{\boldsymbol{\sigma}} = \mathbf{E} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{pl}) \tag{21}$$

Such that the cauchy stress tensor can be realted to the effective stress tensor as follows:

$$\boldsymbol{\sigma} = (1 - \mathbf{D})\bar{\boldsymbol{\sigma}} \tag{22}$$

The nature of the damage evolution is assumed to be a function of the effective stress and the equivalent plastic strain, $\bar{\boldsymbol{\epsilon}}^{\boldsymbol{pl}}$:

$$\mathbf{D} = \mathbf{D}(\bar{\boldsymbol{\sigma}}, \bar{\boldsymbol{\epsilon}}^{\boldsymbol{pl}}) \tag{23}$$

In this formulation, the brittle nature of rock neccessitates seperate characterization of tensile and compressive damage. In the case where a rock sample fails completely in tension, (i.e. the tensile stiffness becomes effectively 0), the compressive strength remains intacts to a fairly high degree such that two seperate damage variables for tensile damage and compressive damage. As such, the equivalent plastic strain is also considered seperately for tension and compression and is represented as follows:

$$\bar{\boldsymbol{\epsilon}}^{\boldsymbol{pl}} = \begin{bmatrix} \bar{\boldsymbol{\epsilon}}_{\boldsymbol{t}}^{\boldsymbol{pl}} \\ \bar{\boldsymbol{\epsilon}}_{\boldsymbol{c}}^{\boldsymbol{pl}} \end{bmatrix} \tag{24}$$

The evolution of the equivalent plastic strains are described by the time derivative of the equivalent plastic strain, which can be considered to be related to the time derivative of the plastic strain through a hardenbing rule, $\mathbf{h}$ such that:

$$\dot{\bar{\boldsymbol{\epsilon}}}^{\boldsymbol{pl}} = \mathbf{h}(\bar{\boldsymbol{\sigma}}, \bar{\boldsymbol{\epsilon}}^{\boldsymbol{pl}}) \bullet \dot{\boldsymbol{\epsilon}} \tag{25}$$

The flow rule can be written in terms of the flow potential function, $G(\bar{\boldsymbol{\sigma}})$, and a plastic mulitplier $\dot{\lambda}$:

$$\dot{\boldsymbol{\epsilon}} = \dot{\lambda}\frac{\partial G(\bar{\boldsymbol{\sigma}})}{\partial \bar{\boldsymbol{\sigma}}} \tag{26}$$

Non-associated plasticity is used, which required the solution of non-symetric equations.

6.1 Damage Evolution and Stiffness Degredation

The evolution of the equivalent plastic strains are formulated by assuming the stress-strain curves can be converted into stress vs plastic strain curves where the tensile and compressive stresses are streated seperately:

$$\begin{aligned} \boldsymbol{\sigma}_t &= \boldsymbol{\sigma}_t(\bar{\boldsymbol{\epsilon}}_{\boldsymbol{t}}^{\boldsymbol{pl}}, \dot{\bar{\boldsymbol{\epsilon}}}_{\boldsymbol{t}}^{\boldsymbol{pl}}) \\ \boldsymbol{\sigma}_c &= \boldsymbol{\sigma}_c(\bar{\boldsymbol{\epsilon}}_{\boldsymbol{c}}^{\boldsymbol{pl}}, \dot{\bar{\boldsymbol{\epsilon}}}_{\boldsymbol{c}}^{\boldsymbol{pl}}) \end{aligned} \tag{27}$$

Loading a quasi-brittle in compression or tension causes damage in the material, which reduces the effective stiffness, weakening the unloading response. This damage is characterized by two damage variables, one of which represents the damage due to tensile loading, the other represents damage due to compressive loading.

$$\begin{aligned} D_t &= D_t(\bar{\boldsymbol{\epsilon}}_{\boldsymbol{t}}^{\boldsymbol{pl}}), \qquad 0 \leq D_t \leq 1 \\ D_c &= D_c(\bar{\boldsymbol{\epsilon}}_{\boldsymbol{c}}^{\boldsymbol{pl}}), \qquad 0 \leq D_t \leq 1 \end{aligned} \tag{28}$$

The damage in both compression and tension is a neccesarily increasing function of the equivalent plastic strains. This formulation will adopt the convention where $\boldsymbol{sigma_c}$ is positive in compression, as with the respectiove strains.

$$\begin{aligned} \boldsymbol{\sigma}_t &= (1 - D_t)\mathbf{E} : (\boldsymbol{\epsilon_t} - \bar{\boldsymbol{\epsilon}}_{\boldsymbol{t}}^{\boldsymbol{pl}}) \\ \boldsymbol{\sigma}_c &= (1 - D_c)\mathbf{E} : (\boldsymbol{\epsilon_c} - \bar{\boldsymbol{\epsilon}}_{\boldsymbol{c}}^{\boldsymbol{pl}}) \end{aligned} \tag{29}$$

For cyclic loading, both the compressive and tensile damage need to be considered. Two stiffness recovery factors are introduced, s_t and s_c, which represent the stiffness recovery effects associated with stress reversals. The damage can be said to take the form of:

$$(1 - D) = (1 - s_t D_c)(1 - s_c D_t), \qquad 0 \leq s_t, s_c, \leq 1 \tag{30}$$

In the case of tensile loading followed by compressive loading, the stiffness is assumed to completely recover

6.2 Governing equations of the coarse-scale (continuum) model

Consider the dynamic equilibrium of a naturally fractured rock mass Ω. Let Γ denote the boundary of Ω and let Γ be divided into mutually exclusive sets Γ_u and Γ_t. The body contains a set of natural fractures denoted by Γ_{cr} and is subjected to a body force $\mathbf{g}$. Let material points in the the undeformed and the deformed configuration be denoted by $\mathbf{X}$ and $\mathbf{x}$, respectively. Let $\mathbf{u}(\mathbf{X}, t) = \mathbf{x}(\mathbf{X}, t) - \mathbf{X}$ denote the displacement of material point $\mathbf{x}$ at time t. Equilibirum of Ω is governed by

$$\rho_s \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{g}, \ \forall \mathbf{x} \in \Omega, t \geq 0, \tag{31}$$

in which $\ddot{\mathbf{u}} = \ddot{\mathbf{u}}(\mathbf{x}, t)$ denotes the second partial derivative of the displacement field and ρ_s is the density of the rock mass.

6.3 FEM Forumulation

7 Constitutive Relationship Parameter Estimation

7.1 Levenburg-Marquardt Algorithm

7.2 Parameter Initial and Boundary Estimates

8 Conclusions

References