1 Abstract

Discrete Element Methods (DEM) explicitly and accurately model the mechanics of naturally occurring 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 is 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. 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 behaviour of various DEM RVE simulations is computed. Subsequently, a CDM constitutive relationship fitted using Levenberg-Marquardt Algorithm (LMA) and the homogenized DEM simulation data. The CDM model is then used in reservoir scale simulations. The CDM model is implemented in ABAQUS^{TM} and DEM simulations were conducted using UDEC^{TM}. The up-scaling methodology is demonstrated through a case study on a naturally fractured carbonate reservoir; the up-scaled CDM model is compared to direction numerical simulation with the DEM model.

2 Introduction

Short paragraph defining homogenization and how it can be used to development a better understanding of rock mechanics. Statement about gap in the literature addressed in this article, i.e., not yet applied to HF.

Discussion of the natural fractured rocks as a multiscale material.

Brief discussion of literature describing multiscale (upscaling) modelling methods. Concurrent vs hierarchical multiscale analysis. See my review article on my website and [Gracie and Belytschko(2011)Gracie, and Belytschko]. Justify that a hierarchical approach is preferable here, do to long simulated time; concurrent approach is to restrictive in terms of time step size. Also justify/explain selection of homogenization instead of an alternative method of upscaling.

Discussion of literature around modeling using homogenization.

- Continuum to continuum and DEM to Continuum. rigid versus deformable particals
- Analogy to debonding of particle -¿ note lack of contact.
- What are the common characteristics of the models.
- What are the unique characteristics of the models.

Overview of DEM literature with a focus on HF
Outline of the article

3 Distinct Element Method

4 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:

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

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

4.1 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$^{\mathrm{TM}}$, 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

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

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

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

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

4.2 Strain Homogenization

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

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

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

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

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

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

5 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.

5.1 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

5.2 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.

5.3 FEM Forumulation

6 Constitutive Relationship Parameter Estimation

6.1 Levenburg-Marquardt Algorithm

6.2 Parameter Initial and Boundary Estimates

7 Material Testing Example

8 Results

9 Conclusions

References

[Gracie and Belytschko(2011)Gracie, and Belytschko] Gracie, R.; Belytschko, T. *International Journal for Numerical Methods in Engineering* **2011**, *86*, 575–597.