

# 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 time 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<sup>TM</sup> and DEM simulations were conducted using UDEC<sup>TM</sup>. 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 -i note lack of contact.
- What are the common characteristics of the models.
- What are the unique characteristics of the models.

### 3 Distinct Element Method

## 4 Homogenization Approach

### 4.1 Stress Homogenization

$$\langle \boldsymbol{\sigma} \rangle^\Omega = \frac{1}{A} \int_\Omega \boldsymbol{\sigma} dA \quad (1)$$

$$\langle \boldsymbol{\sigma} \rangle^\Omega = \frac{1}{A} \left[ \int_{\Omega_r} \boldsymbol{\sigma} dA_r + \int_{\Omega_f} \boldsymbol{\sigma} dA_f \right] \quad (2)$$

$$\langle \boldsymbol{\sigma} \rangle^\Omega = \frac{1}{A} \left[ \sum_{i=1}^{N_b} \boldsymbol{\sigma}^i A_b^i + \sum_{i=1}^{N_d} \boldsymbol{\sigma}^i A_d^i \right] \quad (3)$$

$$\langle \boldsymbol{\sigma} \rangle^\Omega = \frac{1}{A} \left[ \sum_{i=1}^{N_b} \sum_{j=1}^{N_z} \boldsymbol{\sigma}_z^{ij} A_z^{ij} + \sum_{i=1}^{N_d} p_d^i \mathbf{I} A_d^i \right] \quad (4)$$

### 4.2 Strain Homogenization

$$\boldsymbol{\epsilon} = \frac{1}{2} \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] \quad (5)$$

$$\langle \boldsymbol{\epsilon} \rangle^\Omega = \frac{1}{A} \int_\Omega \boldsymbol{\epsilon} dA \quad (6)$$

$$\langle \boldsymbol{\epsilon} \rangle^\Omega = \frac{1}{A} \left[ \int_{\Omega_r} \boldsymbol{\epsilon} dA_r + \int_{\Omega_f} \boldsymbol{\epsilon} dA_f \right] \quad (7)$$

$$\langle \boldsymbol{\epsilon} \rangle^\Omega = \frac{1}{2A} \left[ \int_{\Omega_r} \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] dA_r + \int_{\Omega_f} \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] dA_f \right] \quad (8)$$

$$\langle \boldsymbol{\epsilon} \rangle^\Omega = \frac{1}{2A} \left[ \oint_{\Gamma_r} [\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u}] d\Gamma_r + \oint_{\Gamma_f} [\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u}] d\Gamma_f \right] \quad (9)$$

$$\langle \boldsymbol{\epsilon} \rangle^\Omega = \frac{1}{2A} \left[ \sum_{i=1}^{N_{rb}} [\mathbf{u}_{rb}^i \otimes \mathbf{n}_{rb}^i + \mathbf{n}_{rb}^i \otimes \mathbf{u}_{rb}^i] L_{rb}^i + \sum_{i=1}^{N_{db}} [\mathbf{u}_{db}^i \otimes \mathbf{n}_{db}^i + \mathbf{n}_{db}^i \otimes \mathbf{u}_{db}^i] L_{db}^i \right] \quad (10)$$

## 5 Damage Plasticity Model For Quasi-Brittle Materials

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

$$\epsilon = \epsilon^{el} + \epsilon^{pl} \quad (11)$$

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

$$\dot{\epsilon} = \dot{\epsilon}^{el} + \dot{\epsilon}^{pl} \quad (12)$$

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

$$\sigma = (1 - \mathbf{D})\mathbf{E} : \epsilon^{el} \quad (13)$$

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

$$\mathbf{E}^d = (1 - \mathbf{D})\mathbf{E} \quad (14)$$

Substituting 11 and 14 into 13 results in the following:

$$\sigma = \mathbf{E}^d : (\epsilon - \epsilon^{pl}) \quad (15)$$

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

$$\bar{\sigma} = \mathbf{E} : (\epsilon - \epsilon^{pl}) \quad (16)$$

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

$$\sigma = (1 - \mathbf{D})\bar{\sigma} \quad (17)$$

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

$$\mathbf{D} = \mathbf{D}(\bar{\sigma}, \bar{\epsilon}^{pl}) \quad (18)$$

In this formulation, the brittle nature of rock necessitates separate 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 intact to a fairly high degree such that two separate damage variables for tensile damage and compressive damage. As such, the equivalent plastic strain is also considered separately for tension and compression and is represented as follows:

$$\bar{\epsilon}^{pl} = \begin{bmatrix} \bar{\epsilon}_t^{pl} \\ \bar{\epsilon}_c^{pl} \end{bmatrix} \quad (19)$$

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 hardening rule,  $\mathbf{h}$  such that:

$$\dot{\bar{\epsilon}}^{pl} = \mathbf{h}(\bar{\sigma}, \bar{\epsilon}^{pl}) \bullet \dot{\epsilon} \quad (20)$$

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

$$\dot{\epsilon} = \dot{\lambda} \frac{\partial G(\bar{\sigma})}{\partial \bar{\sigma}} \quad (21)$$

Non-associated plasticity is used, which required the solution of non-symmetric 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 treated separately:

$$\begin{aligned} \sigma_t &= \sigma_t(\bar{\epsilon}_t^{pl}, \dot{\bar{\epsilon}}_t^{pl}) \\ \sigma_c &= \sigma_c(\bar{\epsilon}_c^{pl}, \dot{\bar{\epsilon}}_c^{pl}) \end{aligned} \quad (22)$$

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.

$$\begin{aligned} D_t &= D_t(\bar{\epsilon}_t^{pl}), & 0 \leq D_t \leq 1 \\ D_c &= D_c(\bar{\epsilon}_c^{pl}), & 0 \leq D_c \leq 1 \end{aligned} \quad (23)$$

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

$$\begin{aligned} \sigma_t &= (1 - D_t) \mathbf{E} : (\epsilon_t - \bar{\epsilon}_t^{pl}) \\ \sigma_c &= (1 - D_c) \mathbf{E} : (\epsilon_c - \bar{\epsilon}_c^{pl}) \end{aligned} \quad (24)$$

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:

$$(1 - D) = (1 - s_t D_c)(1 - s_c D_t), \quad 0 \leq s_t, s_c, \leq 1 \quad (25)$$

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  $\Omega$ . Let  $\Gamma$  denote the boundary of  $\Omega$  and let  $\Gamma$  be divided into mutually exclusive sets  $\Gamma_u$  and  $\Gamma_t$ . The body contains a set of natural fractures denoted by  $\Gamma_{cr}$  and is subjected to a body force  $\mathbf{g}$ . Let material points in 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  $t$ . Equilibrium of  $\Omega$  is governed by

$$\rho_s \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{g}, \quad \forall \mathbf{x} \in \Omega, t \geq 0, \quad (26)$$

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

## 5.3 FEM Formulation

# 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.