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## Reservoir rock chemo-mechanical alteration quantified by triaxial tests and implications to fracture reactivation

Zhuang Sun<sup>a,\*</sup>, D. Nicolas Espinoza<sup>a</sup>, Matthew T. Balhoff<sup>a</sup><sup>a</sup> Department of Petroleum and Geosystems Engineering, The University of Texas at Austin, 200 E. Dean Keeton, Austin, TX 78712, United States

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## ABSTRACT

CO<sub>2</sub> injection into geological formations shifts the geochemical equilibrium between the minerals and resident brine. The induced mineral-brine-CO<sub>2</sub> reactions can alter the reservoir rock strength and deformational behavior, which subsequently affects CO<sub>2</sub> storage mechanical integrity. This study attempts to investigate quantitatively the effect of mineral cement and particle dissolution through numerical modeling and validation of triaxial tests performed on unaltered and geologically altered Entrada Sandstone. We utilize a numerical model that couples the discrete element method (DEM) and the bonded-particle model (BPM) to perform simulations of triaxial tests on synthetic rocks that mimic tested rock samples under various confining stresses. Numerical results, in agreement with experimental evidence, show that both cement and particle dissolution significantly contribute to rock weakening in sandstone samples with carbonate/hematite cements and pore-filling carbonate. Sensitivity analyses show that the brittleness of DEM numerical samples is mostly conditioned by the cement bond size among all cement microscopic parameters. An alteration path that mimics the mineral dissolution under subsurface boundary conditions leads to (1) vertical compaction and horizontal stress relaxation in the reservoir rock and (2) transfer of stresses to adjacent strata that results in bond breakage and potentially natural fracture reactivation at a large scale.

### 1. Introduction

Carbon dioxide (CO<sub>2</sub>) capture and sequestration in deep geological formations is a technology proposed to curb carbon emissions to the atmosphere.<sup>1</sup> Although CO<sub>2</sub> injection and enhanced oil recovery are viewed as mature technologies in the oil and gas industry, investigation of all possible implications is necessary for secure and effective long-term CO<sub>2</sub> storage.<sup>2,3</sup> The dissolution of CO<sub>2</sub> into resident brine induces rock-brine-CO<sub>2</sub> interactions that may result in subsequent mineral dissolution/precipitation and clay fabric alteration.<sup>4–7</sup> These chemical reactions can modify rock petrophysical and geomechanical properties.<sup>8–10</sup>

Reaction kinetics of CO<sub>2</sub>-related alteration is dependent on rock mineralogy. Carbonates are more susceptible to rapid mineral dissolution than siliceous minerals.<sup>4,6,11,12</sup> Predominantly quartzitic sandstone samples are not significantly altered by the exposure to CO<sub>2</sub> due to a lack of reactive minerals. On the contrary, sandstone samples with reactive intergranular cements are highly susceptible to CO<sub>2</sub>-induced chemo-mechanical alteration, as minor alterations can result in a large change in geomechanical properties. Examples include carbonate-cemented sandstone (e.g. Entrada Sandstone, Castlegate Sandstone) and

clay-cemented sandstone (e.g., Tuscaloosa Sandstone, Mt. Simon Sandstone). Dissolution of load-bearing mineral phases leads to (1) changes in porosity and permeability, (2) reduction of skeleton stiffness, (3) reductions of fracture toughness, cohesive strength and yield stress locus, and (4) increases of creep compliance.<sup>12–21</sup> The impact of CO<sub>2</sub>-induced mechanical alteration in part depends on the spatial distribution of reactive minerals and position in the granular skeleton, e.g., contact cement, pore filling, and rock matrix.<sup>22</sup>

Triaxial tests provide a tool to evaluate the rock mechanical properties, such as stiffness parameters and shear strength. Brittleness is another mechanical property that characterizes the rock failure process, induced seismicity, and therefore the structural integrity of host formations. Various types of rock brittleness indices have been reviewed in the literature.<sup>23–26</sup> Meng et al.<sup>27</sup> proposed a brittleness index based on post-peak stress-strain curves, which can be readily obtained from triaxial tests. The brittleness index verified by uniaxial and triaxial tests on different types of rock can reflect the influence of confining stress on rock brittleness.<sup>27</sup> At similar levels of confining stress, a transition of brittle to ductile failure mode may appear with successive acid treatments.<sup>17</sup> Numerical modeling on micro-scratch tests shows that the dissolution of interparticle contact cement results in a reduction of brittleness.<sup>28</sup>

\* Corresponding author.

E-mail address: [zhuangsun@utexas.edu](mailto:zhuangsun@utexas.edu) (Z. Sun).

Fault activation and induced seismicity resulting from CO<sub>2</sub> storage are issues related to fluid waste disposal in the subsurface.<sup>3,29–32</sup> Unexpectedly high magnitude microseismic events up to  $M = 1.2$  have been observed in the Decatur project.<sup>33</sup> Mineral dissolution during CO<sub>2</sub> sequestration can induce reservoir compaction and stress relaxation; in extreme scenarios mineral dissolution may cause a compaction-driven shear failure of the reservoir.<sup>34–36</sup> Hence, coupled chemo-mechanical processes can contribute to further stress changes in subsurface storage formations, which would result in additional fracture reactivation and potential induced seismicity.

This study presents a model based on the DEM to investigate the mechanical behavior of cemented sandstone samples susceptible to interparticle contact cement and particle dissolution. First, we present an overview of the DEM-BPM numerical model and introduce a brittleness index. Second, we explore the role of mineral dissolution of cements and particles on mechanical properties of CO<sub>2</sub>-altered rocks through comparison of simulated and experimental data from triaxial tests. Last, we discuss how the mineral dissolution affects change of local stresses in the reservoir and in adjacent strata that may lead to fracture reactivation.

## 2. Methods

### 2.1. Discrete element method-bonded-particle model

The discrete element method (DEM) has been widely used to study the mechanical behavior of granular media.<sup>37</sup> Potyondy and Cundall<sup>38</sup> proposed the bonded-particle model (BPM) to simulate rock mechanical behavior with cemented granular media. The DEM-BPM relates particles and bonds to grains and cements observed in sedimentary rocks. Micromechanisms that define small and large strain rock behavior may be difficult and complex to capture by existing continuum approaches and constitutive relations. DEM-BPM imposes no theoretical assumptions and limitations on material properties and thus the macroscopic behavior emerges from a set of micromechanical properties for the grains and cements. For instance, in the DEM-BPM, a macroscopic fracture automatically forms due to the interaction and coalescence of broken bonds. The DEM-BPM simulations performed in this study utilize the discrete element code LIGGGHTS.<sup>39</sup>

The cemented sandstone is simulated as bonded spherical particles in the DEM-BPM. Particles interact via contacts that possess finite normal and shear stiffnesses. The mechanical behavior of the entire system arises from the interaction of particles and force/moment exerted at each contact. Newton and Euler equations relate the particle motion and the resulting forces and moments. Bonds at contacts confine the relative displacements and rotations of bonded particles. Bonds can break when either the normal or shear stress exceeds the threshold strength. The DEM-BPM assumes that (1) particles are rigid spheres with finite mass, (2) particles interact only at contacts, and (3) force-displacement laws at contacts permit calculating the resultant force and moment for particle motions.<sup>38</sup> The bond size is a local parameter that can be related to the sizes of the bonded particle pair.<sup>40</sup> Hence, we adopt a dimensionless coefficient  $\lambda$ , which defines bond size everywhere in the domain. Such that for two arbitrary bonded particles  $i$  and  $j$  with radii  $R_i$  and  $R_j$ , the radius of the bond is:

$$R_{b,ij} = \lambda \frac{R_i + R_j}{2} \quad (1)$$

Parameter  $\lambda$  ranges from 0 (no cementation) to 1 (full cementation). Fig. 1 illustrates the DEM-BPM model in two dimensions. The reader can find the detailed formulations elsewhere.<sup>41,42</sup>

Macroscopic behavior of the entire system depends on the micromechanical properties of grains and cements, i.e., particles and bonds in the DEM-BPM. The force and moment acting at bonded particle contact result from a force of particle-particle contact and a force and moment transferred by the bond. We calculate the forces and moments between

particles by introducing independent microscopic parameters. Each bonded particle contact has a local frame that is decomposed into the normal direction along the bond element and tangential directions. Micromechanical properties of particles include elastic modulus  $E$ , stiffness ratio  $k_T/k_N$ , grain mass density  $\rho$ , and friction coefficient  $\mu$ . Slippage occurs when the tangential force exceeds the limit defined through the local friction coefficient  $\mu$ . The bonds are elastic materials with limited values for displacements and rotations. Micromechanical properties of bonds include bond elastic modulus  $E_b$ , bond stiffness ratio  $\bar{k}_T/\bar{k}_N$ , bond size parameter  $\lambda$ , bond normal strength  $\sigma_c$  and shear strength  $\tau_c$ . Bond breakage is determined by the stress state of  $\sigma_{\text{normal}} > \sigma_c$  or  $\tau_{\text{shear}} > \tau_c$ , all in [Pa] unit. Bond local stresses  $\sigma_{\text{normal}}$  and  $\tau_{\text{shear}}$  are conditioned by the bond stiffness related to  $E_b$ ,  $\bar{k}_T/\bar{k}_N$  and  $\lambda$ . Bond strength  $\sigma_c$  and  $\tau_c$  set stress limits for the bond breakage. We assume that particles and bonds possess the same elastic modulus and stiffness ratio to reduce the number of free parameters. Particle density is  $\rho = 2650 \text{ kg/m}^3$  and friction coefficient is  $\mu = 0.5$ .

### 2.2. Brittleness index

Brittleness characterizes rock failure and creation of new failure surfaces. An increase of mean effective stress, temperature and loading duration can result in failure transition from brittle to ductile.<sup>43–46</sup> Meng et al.<sup>27</sup> proposed a brittleness index  $BI_p$  based on post-peak triaxial stress-strain curves:

$$BI_p = BI_{p1}BI_{p2} = \frac{\tau_p - \tau_r}{\tau_p} \frac{\log_{10} \left| \frac{k_{ac}}{MPa} \right|}{10} \quad (2)$$

where  $BI_{p1}$  is the magnitude of the relative post-peak stress drop and  $BI_{p2}$  represents the velocity of stress decrease. Parameters  $\tau_p$  and  $\tau_r$  are the peak and residual stresses, respectively. Parameter  $k_{ac}$  is the slope of the line that joins the peak strength point to the starting point of the residual strength. Both  $BI_{p1}$  and  $BI_{p2}$  range from 0 to 1. The form of  $BI_{p2}$  is to normalize the value of  $k_{ac}$  within the range of 0–1. A larger value of  $BI_{p1}$  and  $BI_{p2}$  results in a larger  $BI_p$ , indicating a higher brittleness. The index  $BI_p$  is suitable to evaluate rock brittleness with uniaxial and triaxial tests on various types of rock.<sup>27</sup>

## 3. Results

### 3.1. Experimental triaxial data

Espinoza et al.<sup>10</sup> performed triaxial tests on Entrada Sandstone air-dry samples at confining stress  $\sigma_3 = 0.69 \text{ MPa}$  (100 psi), 6.9 MPa (1000 psi) and 20.7 MPa (3000 psi). Samples are 25 mm in diameter and 54 mm in height. CO<sub>2</sub>-altered and unaltered Entrada Sandstone samples were taken from outcrops in the Crystal Geyser field that has been used as a CO<sub>2</sub> sequestration analog. CO<sub>2</sub>-altered samples are subject to hematite dissolution, which leads to the bleaching of otherwise red unaltered samples. Thin section and micro-tomography analyses showed higher porosity and less cementation in altered sandstone than unaltered sandstone. Entrada Sandstone has a grain size distribution mostly in the range of 50–100  $\mu\text{m}$ .

### 3.2. Baseline unaltered Entrada Sandstone model and calibration

The DEM numerical sample is initialized as a random particle packing with a uniform diameter distribution from 50 to 100  $\mu\text{m}$ . The cylindrical DEM numerical sample has a height of 2.54 mm and a diameter of 1.27 mm, containing 7928 particles and 23,178 bonds. The porosity is 39%, not including cement bond volume. Similar to the experimental conditions, we apply different constant confining stresses,  $\sigma_3 = 0.69 \text{ MPa}$ , 6.9 MPa and 20.7 MPa in the radial direction. We apply the constant confining stress through  $10 \times 12$  segmented servo walls in the radial direction. (Fig. 2)

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