



A parallel-bonded chemical corrosion model for discrete element modelling of chemically corroded limestone

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ABSTRACT

The mechanical behaviours of rock mass are influenced by the presence of cracks at the microscopic and macroscopic levels. When coupled with corrosion by chemical ions in ground water, these cracks can cause instabilities and fragmentation near the excavated surface of underground structures, such as shield tunnels, *etc.* This paper presents the development of a parallel-bonded chemical corrosion (PCC) model for modelling corroded rocks (limestone). The model extends the bonded-particle model (BPM) by adding a chemically induced damage law to the particle bond. The damage law of the PCC model is derived from Nuclear Magnetic Resonance (NMR) and triaxial compression tests. The PCC model is validated with experimental results and is capable of simulating the micro-damage evolution process as well as predicting the macro-mechanical degradation caused by the chemical corrosion. It is then applied to investigate chemical effects on crack initiation, propagation, coalescence, and the mechanical properties of the limestone containing pre-existing flaws. Microscale correlations are derived linking the crack propagation process, flaw distribution and the effects of chemical corrosion.

1. Introduction

Deep subsurface rock mass is often surrounded by water, which contains complex chemical ions that may have different pH values. At the macroscopic level, chemical damage causes various extents of reduction in mechanical properties [1]. At the microscopic level, rock can be viewed as an assemblage of mineral grains, which are often anisotropic in both modulus and strength [2]. In sedimentary rocks, such as limestone and sandstone, the grains adhere to one another by cementitious materials which can deform, break, or be dissolved by chemical solutions [3]. Rock corrosion caused by water accelerates the failure process, leading to mechanical degradation and geological disasters such as landslides and earthquakes [4].

The mechanical behaviour of rock is also influenced by the presence of discontinuities. Such discontinuities are found at all scales, from grain boundaries to joints and regional faults [5,6]. The existence of discontinuities, such as joints, cracks, *etc.*, in rock mass has two main effects: (1) by reducing the intact section inside rock, these discontinuities decrease the strength of the rock; (2) under

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external stress, new discontinuities may initiate from the existing cracks, and propagate and connect with other cracks, further decreasing the strength of the rock [7,8]. Coupled with chemical effects, the mechanical behavior, and the crack propagation and connection processes may be more complicated. Therefore, it is important to investigate the micro damage caused by chemical effects and the process of crack initiation, propagation, coalescence as well as the failure mechanisms of rock under coupled chemical-mechanical impacts during their use for rock engineering applications, such as tunnels, foundations and slopes, and hydrocarbon and geothermal energy extraction [9].

Over the past few years, considerable laboratory tests have been carried out to investigate the macroscopic and microscopic mechanical properties of rock without pre-existing cracks and under various chemical environments [10–13,5,14–16]. However, it is still very difficult for real-time monitoring of laboratory experiments designed to quantitatively analyse the chemical corrosion process of rock while subjected to loading. To have a better understanding of crack initiation, propagation and coalescence processes during external rock compression, indirect techniques, such as acoustic emission (AE) [17–19], computerised tomography (CT) scan [20–22], microscopic observation (petrographical thin section, SEM/ESEM) and high-speed camera are sometimes used [23].

In physical lab tests, the detection of crack propagation of rock samples with pre-existing flaws, especially for crack initiation, is based on the first distinct cracking sound or the first minute crack opening observed on the specimen surface. However, as shown in other experimental studies employing AE [24] and CT [25] techniques, cracking events prior to those observed on the surface may occur inside the rock specimens. Even when shear failure bands can be distinguished, the AE and CT resolution is often too low to capture the development of distinct crack trajectories [26,27].

Numerical modelling of rock mechanics and rock engineering processes enables easier and detailed investigation and visualization of micro cracks, stress distributions and other variables [28–32]. Using extended finite element method (XFEM), Mohtarami et al., [33] conducted three - point and four - point bending tests on chemically corroded rock samples to investigate the crack propagation law. The results show that the deformability of the sample increase with the growth of the chemical ions concentration; fracture toughness of the sample decrease with the growth of pH values of the solutions. Abdelghani et al., [34] used Hydro-Geosphere, a numerical tool, to analyze unsaturated water flow in an open pit filled with mining wastes. This involved water flow and solute transport effects associated with recharge, waste material and fractures of the in the surround rock mass.

Discrete Element Method (DEM) is a rapidly developing area in computational mechanics. This modelling approach which represents rock as an assemblage of particles (spheres, ellipsoids, blocks) that interact with each other, has been recognised as both a scientific tool and an engineering tool to investigate the mechanic properties of rock in both microscopic and macroscopic scales [35]. Bonded particle model (BPM), based on DEM, constitutes a dense packing of non-uniform sized circular or spherical particles [36]. All particles are bonded together by bonds that have specific stiffness and strength. These particles can be detached when external loads exceed the bond strength [37].

BPM is widely used for modelling the mechanical behavior of rock. Asadi et al., [38] conducted direct shear tests by using BPM to simulate the fracture of synthetic rocks and to investigate the effect of micro-properties shear fracture. Different kinds of failure including asperity sliding, cut-off, and asperity degradation were explicitly observed and evaluated. Zhang et al., [39] used BPM to investigate pore size and distribution effects on the uniaxial compressive strength (UCS) of lithophysal rocks. Their results show that UCS decreases when pore radii increase but decreases due to the existence of pores with the same condition of porosity. Most previous studies focus on mechanical properties such as elastic and plastic deformations, and failure mechanisms of intact rocks [40,41], or the relationship between modelling parameters and mechanical properties of intact rocks [42]. Research on the micro damage investigation and the crack propagation of chemically corroded rock using BPM in DEM is rare.

This paper presents a parallel-bonded chemical corrosion (PCC) model, which extends the features of the bonded-particle model (BPM) by adding a damage evolution law to the parallel bond. Limestone is used as an example rock type. Before mimicking the chemical corrosion processes using the PCC model in DEM, laboratory chemical corrosion tests on limestone are first conducted to investigate the micro damage evolution using Nuclear Magnetic Resonance (NMR). Internal microstructure images and T_2 values (transverse relaxation time distribution, which depends on the size of water-saturated pores) for chemically corroded limestone are obtained. Based on the experimental data, a micro damage cumulative model of the corroded limestone is proposed and then implemented in the BPM (with parallel bond) to form the PCC model. The PCC model is applied for DEM simulations to investigate chemical effects on crack initiation, propagation, coalescence, and the mechanical properties of the limestone containing pre-existing flaws. Microscale correlations are derived linking the crack propagation process, flaw distribution and the effects of chemical corrosion.

2. Micro damage evolution in chemical corroded limestone

2.1. Experimental methods

Microscopic damage is the root cause of macroscopic mechanical degradation. To quantify damage at the microscale and construct the micro damage model of the rock during chemical corrosion, a damage variable must be defined. In this paper porosity is selected as the key parameter of the damage variable D , calculated as [44]:

$$D = \frac{V - V_D}{V} = \frac{n - n_0}{1 - n_0} \quad (1)$$

where, D is the damage variable, V is the volume of the sample, V_D is the volume of the damaged part of the sample, n_0 is the porosity of the sample in air, and n is the porosity of the sample after being subjected to external damage, such as chemical corrosion or loads.

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