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Research Paper

Mechanical deterioration of rock salt at different confinement levels: A grain-based lattice scheme assessment

Ning Liu [a], Min Li [a], Weimin Chen [b,*]

[a] School of Aeronautics Sciences and Engineering, Beijing University of Aeronautics and Astronautics, Beijing 100191, China
[b] Key Laboratory for Mechanics in Fluid Solid Coupling System, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China

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ABSTRACT

A two-dimensional gain-based lattice approach, is developed here, driven by the needs for modelling strategy of rock salt (halite). In this scheme, considering crystalline micro-structure, halite is discretized into polygonal grains by smooth joint logic, in which mass nodes with micro-rotation are connected by springs. The contacts between grains are in a point-to-point manner, which can avoid complex contact definition (point-to-edge, or edge to edge, etc.) in classical numerical simulations. Breakage and creation of interactions in dynamic spring network is applied to implement the dislocation and diffusion within grains in addition to crystal plasticity.

Brazilian tensile test, unconfined and triaxial compression tests are presented for a guideline of parameter identification and a consistent simulation set-up. Relatively comparable results including brittle-ductile transition could be reproduced, revealing the potential to study and quantify the interplays of mechanical deterioration of halite.

1. Introduction

Rock salt is also known as halite, which is a kind of salt and exhibits isometric crystal structure. It was found to have a low permeability and porosity [1,2], excellent sealing capacity of faults [3] and possess a creep behaviour under a low stress level [2]. Due to those incredible characteristics, rock salt has been widely used in many fields. For instance, early engineering studies of rock salt were driven largely by the need to design safe salt mines [2]. Then, it was applied into oil or hydrocarbon gas storage [4], and even it was considered to have the possibility to host a deep geological repository for radioactive, high-level waste from nuclear facilities [5], such as Waste Isolation Pilot Plant of USA [6]. Based on the economic and environment-friendly importance, in order to provide a scientific basis for proper stability evaluation and safe design, construction and operation, it's necessary for us to study deeply on halite rocks.

In recent decades, scholars and researchers have made a lot of efforts from the perspectives of experimental tests, theoretical analysis and numerical simulation, which have influenced positively on current research and future potential applications. Experimental measurement is a kind of direct methodology. Some static and dynamic material parameters of rock salt specimens were obtained by this method [7–11]. Time [2,12,13] and temperature [14,15] dependent properties were observed and studied in the past. As for the aspect of theoretical studies, some mathematical models and contact laws were developed based on the in-situ measurements and laboratory tests to predict short-term as well as long-term mechanical responses [16–19]. Nevertheless, numerical simulation may be regarded as a bridge between theoretical methods and experiments. It could provide valuable reference data and prediction for engineering design or practical applications in a more economic and efficient way. Additionally, it may complete some experiments which are hard or even impossible to cope with by other approaches [20]. With the great improvement of computer performance, numerical methods are playing an increasingly important role in the current research. For salt-rock, exploration of advisable constitutive models and modelling strategy is still an ongoing task [21].

Generally, the numerical simulations could be further divided into two categories: continuum and dis-continuum based methods. Within continuum researches, as early as 1989, Evans and Nunn [22] used the finite difference method (FDM) assessed the driving convection mechanisms near salt dome [22]; In 1998, FDM was used to model the development of the salt structure [23]. Also, finite element method (FEM) has been applied to study the mechanical properties of rock salt. For example, in 1972, based

* Corresponding author.
E-mail address: wmchen@imech.ac.cn (W. Chen).

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on FEM, Thoms et al. [24] tried to model the creep behaviour of rock-salt pillar samples for predicting the closure of rooms in salt domes or bedded salt [24]; recently, Moghadam et al. [25] utilized elasto-visco-plastic constitutive model into FEM equations to explore the dilatancy, short- and long- term failure of rock salt. While, due to the limitations of the continuum assumptions, these methods may barely handle some problems related to large-scale fractures, complex discontinuities, or microscopic mechanism [26].

Therefore, the dis-continuum based methods, like molecular dynamics (MD) and discrete element method (DEM), were developed. MD, whose basic elements are actual ions, atoms and molecules, mainly deals with the problems at micro- or nano- scale. This scale feature and complex potential functions may limit its research and engineering applications. Based on the initial concept of MD, DEM was first proposed by Cundall [27] to study rocks and other geo-materials. Early, it used bonded particle model, consisting of circular or spherical elements [28], to simulate grains. Obviously, these rounded shape particles are not proper candidates for rock salt simulation, based on halite's physical and chemical micro-structure. For now, polygonal-shaped elements in two-dimensional or three-dimensional have been developed and widely used in the salt-rock study [29,30]. These means could be utilized to capture the inter-crystalline deformation and failure behaviours of rock salt, but it seems to be difficult to simulate the micro-cracks opening, propagation and proliferation within crystalline gains. Besides, the implementation of those methods are so complex that it may highly penalize calculation efficiency [28].

Meanwhile, the concept of lattice models (LM) was established. In theory, lattice models are based on the atomic lattice models of materials [31]. In contrast to DEM, the elements are replaced by point masses instead of spherical particles and the contacts between elements by simple springs or beams. These characteristics make LM flexible to model both granular media and continuum systems [31]. The scale of specimens in research may be extended by a coarser lattice idea (larger than real atomic scale) that could be dated back to Hrennikoff [32]. This model is well suitable to emulate the fractures in rock and other engineering materials. However, it seems to be hard to simulate the cracking or sliding along the grain boundaries, which exactly exist in rock salt.

Based on the physical and chemical nature of salt-rock, a grain-based lattice scheme is developed here, that might be regarded as a kind of granular media with polyhedral elements incorporating micro-rotation and breakage/creation of interactions within crystalline grains. The whole sample is discretized into nodes with given masses connected by normal and shear springs with Mohr-Coulomb criterion. Some points of departure from the available lattice models are the introduction of given micro-rotational inertia independent of lattice spacing, smooth joint logic (SJL) and creation of new interactions. They could be used to control the size-dependent effect, capture grain sliding and implement the dislocation and diffusion within grains in addition to crystal plasticity, respectively.

The aim of this research is to attempt to establish an alternative and promising modelling strategy for rock salt at grain scale in a more realistic and simpler way. A guideline for parameter identification and a consistent simulation procedure is presented. Complementary insights and a deeper understanding of confinement effect on mechanical deterioration are explored systematically and quantitatively from the perspectives of compressive strength, volume changes, fabric tensors and failure modes. The rest of this paper is organized as follows. Firstly, basic methods we used are described in Section 2, including the general idea of lattice approach, a review of the concept of SJL, parameter identification and the calculation process. Then, numerical simulations and results are presented in Section 3 compared with experiments to validate the model and calibrate material parameters by Brazilian tension and uniaxial compression simulations, explore the confining pressure effect by varying confinement levels in biaxial compression tests; also, the capability in predicting mechanical behaviour of rock salt is discussed and evaluated. Finally, some conclusions are highlighted in Section 4.

2. Basic methods

Previously, lattice model was mainly used to model elastic and brittle media [33]. While, some researches show it has the potential to emulate ductile materials [34,35] as well. Therefore, we extend it to represent a kind of cohesive-frictional medium, including brittle-to-ductile transition, rock salt. Lattice networks stand for the interior of crystalline grains, and the SJL accounts for the movements along grain boundaries. The interactions between polygonal grains generated by PolyMesher code [36] are in a simple point-to-point manner, which may take less time consuming than that polyhedral interaction logic in DEM [37]. In particular, the singularity issues involved in the definition of those complex contacts, such as the interactions among facets, edges and points [38], could be avoid [39].

2.1. Interactions in lattice model

A cohesive frictional constitutive law [28] is used to define the interactions between two nodes. This model takes the linear elastic behaviour into consideration, with cohesion and friction, and Mohr-Coulomb plasticity surface is also included.

Under the condition of a small deformation, rock salt behaves elastically and linearly. During that process, contact forces, including normal force F_n and tangential force F_s, for every pair of interaction, are applied here, and the contact model is shown as Fig. 1. Normal force F_n between two nodes, can be written as

$$F_n = k_n \cdot \Delta d, \tag{1}$$

$$\begin{aligned} \Delta d &= d_{eq} - d, \\ d &= \left(\vec{x}_2 - \vec{x}_1\right)\vec{l}_{12}; \end{aligned} \tag{2}$$

where $k_n, d_{eq}, d, \vec{x}_1, \vec{x}_2, \vec{l}_{12}$ is the normal spring stiffness and the equilibrium distance, the distance, coordinate vectors and the normal of the spring between two nodes as shown in Fig. 2, respectively.

In the case of tension, we define a maximum acceptable tensile force $F_{n,max}$. When $d_{rupture} < \Delta d < d_{tensile}$, a soft coefficient k_{sf} is introduced, and then the tensile force F_n can be displayed as

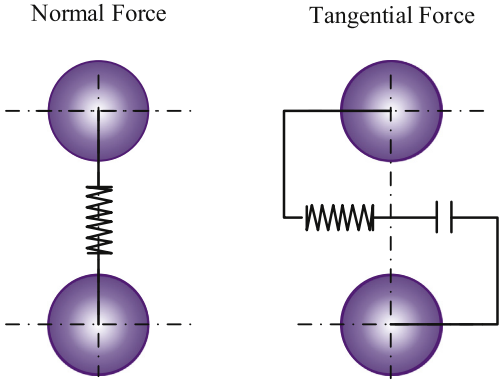

Fig. 1. Constitutive model (including Mohr-Coulomb criterion).