International Journal of Rock Mechanics and Mining Sciences 103 (2018) 230–241

Contents lists available at ScienceDirect

International Journal of Rock Mechanics and Mining Sciences

journal homepage: www.elsevier.com/locate/ijrmms

Modeling deformation and damage of rock salt using the discrete element method

Christian Müller[a,*], Thomas Frühwirt[b], Daniel Haase[c], Roger Schlegel[c], Heinz Konietzky[b]

[a] BGE TECHNOLOGY GmbH, Esc henstraße 55, 31224 Peine, Germany
[b] TU Bergakademie Freiberg, Institut für Geotechnik, Gustav-Zeuner-Straße 1, 09599 Freiberg, Germany
[c] Dynardo GmbH, Steubenstraße 25, 99423 Weimar, Germany

ARTICLE INFO

Keywords:
Rock salt
Excavation damaged zone
Discrete element method
Voronoi
Acoustic emission
Fracture network
Microcracking

ABSTRACT

Rock salt is considered to be a suitable host rock formation for radioactive waste repositories. However, local stress changes caused by drift construction lead to the evolution of an excavation damaged zone (EDZ). Such an EDZ can have a major impact on the safety of a radioactive waste repository because it can violate the integral sealing function due to the development of a permeable microcrack network. The objective of this investigation is the development of a modeling strategy that can be used to simulate the damage behavior of rock salt at grain scale. For this purpose, discrete element modeling techniques were used in combination with polyhedral-shaped elements (Voronoi polyhedra) in order to duplicate the shape and arrangement of grains. To calibrate the material parameters used in the constitutive models and to validate the relevant damage and fracture processes, uniaxial compression tests were combined with acoustic emission measurements. Overall deformation behavior and crack evolution was reproduced by modeling and validated by lab experiments. The new proposed modeling strategy based on DEM and Voronoi polyhedra shows new possibilities to simulate the mechanical behavior of rock salt in a realistic manner by explicitly considering the fracture processes at grain scale.

1. Introduction

Deep geological formations are regarded to be suitable to host repositories for radioactive waste. An important part of the safety concept is the identification of a suitable rock formation that ensures the safe containment of the waste. In addition to claystones and granitic rocks, especially salt formations are suitable to host a deep geological repository for highly radioactive waste.[1] In Germany, the safety concept for a deep geological repository in salt formations considers not only the containment capability of the geological barrier but also that of the geotechnical barriers in order to seal all man-made openings (e.g., shafts, chambers, and drifts).[2] However, local stress changes adjacent to man-made openings lead to the evolution of an excavation damaged zone (EDZ) during and after excavation. Such an EDZ can have a major impact on the operation and sealing of a radioactive waste repository.[3]

The EDZ is a region where microcracks and to some extend also fractures have developed. This decreases the material strength and thus increases the permeability of the initially tight host rock. The initiation of microcracks starts from existing flaws acting as stress concentrators.[4] In crystalline materials, it is widely assumed that grain boundaries act as the predominant source of stress concentrating flaws.[5] With increasing degradation, the coalescence of individual fractures results in a pervasive fracture network where a significant increase in permeability can be observed. The mathematical theory that considers the influence of connectivity on the conductivity is the so-called "percolation theory".[6] Below a certain percolation threshold, the influence of the hydraulic conductivity of individual fractures on the integral permeability is negligible because a continuous path for fluid flow does not exist.[7–9] The percolation theory is also applicable when describing the hydraulic behavior of the EDZ in rock salt.[10,11] The microstructural damage that occurs in the EDZ can therefore violate the integral sealing function of the barrier, even though the geotechnical barrier itself can be regarded as intact. Thus, in a first step a deeper characterization of the fracture network around excavations is necessary in order to assess in a second step the integral hydraulic performance of the barrier.

The numerical methods used in rock mechanics can be generally classified into continuum and discontinuum approaches.[12] In the field of salt mechanics, many methods used to describe the mechanical behavior are based on continuum mechanical approaches where the damage is considered as an isotropic property.[13] Tsang et al.[3] identified several aspects that need to be addressed to enhance the understanding of the EDZ and the modeling techniques to simulate its behavior. An

* Corresponding author.
E-mail address: christian.mueller@bge.de (C. Müller).

https://doi.org/10.1016/j.ijrmms.2018.01.022
Received 2 June 2017; Received in revised form 18 December 2017; Accepted 5 January 2018

area of significant weakness in EDZ studies is that of anisotropy. Boundary conditions and rock properties, such as in-situ stresses, fracture networks or induced permeability changes caused by drift construction are anisotropic and the interaction of these properties and their behavior are an open question.[3] Some efforts were made to consider anisotropic damage inside the EDZ.[14] However, the interaction between damage and permeability cannot be studied explicitly since the solutions are based on continuum approaches where both properties are simply linked by empirical functions. In order to further investigate the initiation, propagation and interaction of fractures, it is necessary to simulate the fracturing in the EDZ explicitly. Therefore, a continuum-based approach is suitable to only a limited extent.

For analyzing and simulating the fracture and damage behavior of rock explicitly, discontinuum approaches, especially the discrete element method (DEM) and related methods (e.g. hybrid continuum-discontinuum approaches) have become increasingly important.[15,16] The basic approach of the DEM is an assemblage of discrete elements and contacts among them establishing the medium. The approach allows an arbitrary displacement and rotation of the discrete elements, a separation of discrete elements along their contacts as well as the detection of new contacts.[17] When considering the shape of the discrete elements, the DEM approaches available are generally divided into particle-based and polygonal-based discrete elements. The Particle Flow Code (PFC) is a well-known particle-based code.[18] It uses circular (2D) or spherical (3D) particles with a non-uniform distribution to simulate the rock structure.[19] However, as revealed by Kazerani and Zhao[20], the use of spheres also has some drawbacks. Grain interlocking, which usually exists in crystalline microstructures is basically neglected due to the rounded particle shape. Several solutions to overcome this difficulty have been developed.[21–23] Another method is the use of polygonal-shaped elements. Several publications show the ability for investigating the failure of rock using polygonal-shaped elements.[24–26] The best-established code is the universal distinct element code (UDEC), which uses convex polygonal- (2D) or polyhedral- (3D) shaped discrete elements.[27] Relatively new in this field are hybrid continuum-discontinuum techniques where virtual smeared cracks embedded in the finite element mesh are transferred into physical discontinuities to simulate the fracturing.[28,29] This approach was also successfully applied to study the fracturing inside the EDZ.[30]

The modeling approaches mentioned above are mainly based on two-dimensional models. However, such an approach contains several limitations, particularly with regard to the complex fracture systems and the associated anisotropic permeability changes. An issue relevant to nuclear repositories is the EDZ extent perpendicular to the drift contour into the host rock. However, the initiation, propagation and interaction of fractures as well as the associated permeability increase must also be studied in three dimensions, because migration of gas and fluids through fractures is also parallel to and not only perpendicular to the drift contour. A grain-based model featuring three-dimensional discrete elements is proposed by Ghazvinian el al.[31] The simulation uses elastic grains (discrete elements) to simulate crack damage development in brittle rock (granite), but these elastic grains are not suitable to simulate the inelastic rheological properties of salt to be considered here. Some effort was made to simulate the mechanical deformation of rock salt on a three-dimensional discontinuum-mechanical basis, where classical laboratory tests were used to validate the computer model.[32] However, only the macroscopic behavior can be validated this way. Therefore, further investigations are necessary to validate the micromechanical fracture mechanisms and the simulated fracture pattern.

The objective of this investigation is primarily aimed at establishing whether the deformation behavior of rock salt and the development of microstructural damage along grain boundaries occurring in the EDZ can be simulated using discontinuum based computer models. For comparison and to validate the computer model it was decided to simulate the fracturing at laboratory scale. Combined acoustic emission and uniaxial compression tests as well as microstructural analyses were carried out to evaluate the macroscopic behavior micromechanically. In order to simulate the shape and arrangement of crystal grains in rock salt, the discrete element method (DEM) was applied using polyhedral elements for the simulation.

2. General modeling strategy

Local stress changes adjacent to man-made openings result in microcracking and granular disintegration during and after excavation. Although this results in a macroscopic deformation, the relevant processes that induce an EDZ occur at the scale of the microstructure. The macroscopic mechanical characteristic of a polycrystalline material is influenced by the mechanical behavior of single crystals as well as the geometric (fabric) structure of the crystals forming the microstructure. The mechanical behavior of single crystals includes the deformation of grains and their boundaries, whereas the fabric includes their arrangement, size and shape. Thus, a first step for grain scale modeling is the accurate construction of a representative microstructure as well as an appropriate tool for simulating the fracture and damage behavior.

2.1. Using the Voronoi tesselation to reconstruct the microstructure

The information obtained from experimental characterization is generally used to reconstruct the microstructure. The reconstruction and generation is based either on deterministic or stochastic approaches. Deterministic approaches use image information gained directly from thin sections to transfer the microstructure onto a grid, e.g. using the mesh of a Finite Element Method (FEM) model or discrete elements using the DEM.[33–35] Stochastic approaches use statistical data obtained from experimental characterization to randomly generate grains with representative sizes and shapes. Especially randomly generated particles, based on the Voronoi tessellation, are in the spotlight of scientific interest.[25,32,36–38] A major advantage of the Voronoi tessellation is the grain shape variability, which is representative for polycrystalline rock samples.[39] Since rock salt consists of individual grains that are connected by grain boundaries forming a polycrystalline microstructure, the Voronoi tessellation was considered as a suitable way for modeling the microstructure.

However, the Voronoi geometry is practically difficult to handle by numerical codes due to potential small polyhedral edges leading to bad-quality zone elements. Moreover, the zone quality controls the critical time step for calculation, and optimization can decrease the calculation time. Therefore, a Voronoi generation library was considered, where the geometry is optimized after generation. The large-scale 3D random polycrystal generator *Neper* proposed by Quey et al.[39] was used, which allows the removal of small-scale entities (edges and faces). This way, geometrically improved Voronoi models could be generated.

Since the microstructure has an influence on the fracture development,[40] it is first verified how well the typical shape and arrangement of rock salt grains is simulated by Voronoi polygons. Comparisons of real and simulated microstructures are based on quantitative image analysis of thin sections of rock salt. Three thin sections were cut perpendicular to each other along the cylindrical axis to allow a comparison with the three-dimensional Voronoi pattern. Visual studies of the thin sections were done using a petroscope (MAP, ADC-3L) and by tracing the grain boundaries. Then, *ImageJ 1.47t* (Wayne Rasband) was used for the quantitative analysis by determining typical microstructural features, e.g. shape and size. Additionally, a cube with an edge length of 10 cm and 15625 elements was generated using the Voronoi algorithm *Neper*,[39] which results in an average Voronoi element edge length of approximately 4 mm. Slices were cut along the principle directions und analyzed in the same way as the real rock samples using *ImageJ* (Fig. 1).

Grain size is the dominant microstructural feature of polycrystalline materials. The diameter of particles is usually based on a certain equivalency criterion. The surface-equivalent sphere diameter was