UNIVERSITY OF PETROȘANI

DOCTORAL SCHOOL

DOCTORAL THESIS

SUMMARY

RESEARCH ON MODELING AND SIMULATION OF THE MECHANICAL CHARACTERISTICS OF LIGNITE USING ADVANCED COMPUTER APPLICATIONS

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2023

Investigating the properties of a rock mass through the application of specific rock mechanics concepts is of paramount importance in mining, civil engineering, hydrotechnical construction, industrial projects, and road construction. Utilizing the theory of continuous mediums, understanding and predicting the behavior of rocks becomes challenging due to their discontinuous, anisotropic, and heterogeneous nature. Knowledge of a rock mass' properties serves as the starting point for anticipating its deformations, both quantitatively and qualitatively.

From the perspective of the extractive industry, whether it be surface or underground mining, understanding the properties of rocks enables the determination of their stability and the establishment of design and execution conditions. Globally, there is a trend towards the use of numerical methods in studying the properties and stresses of rocks, whether dealing with rock masses or samples. These methods complement laboratory determinations when simulating specimen behavior or serve as direct means of assessing mass stability based on rock properties determined in the lab.

Simultaneously, numerical simulations based on virtual models also serve as modern educational tools for understanding the behavior of rocks subjected to various mechanical stresses. For these reasons, within the scope of this doctoral thesis, I have deemed it opportune to address the modelling and simulation of compression, indirect and direct tension, as well as shear stresses for lignite.

I chose lignite as the rock type because, despite decarbonization policies and restrictions on fossil fuel use for energy production, lignite continues to represent and will remain an energy source. Additionally, I considered the fact that known lignite deposits exhibit a wide variability in physico-mechanical properties, which is crucial in selecting and designing machinery for their extraction.

The doctoral thesis is titled "Research on Modeling and Simulation of the Mechanical Characteristics of Lignite Using Advanced Computer Applications" and presents the main scientific, theoretical, and experimental results obtained during the doctoral stage. With the emergence of new research, knowledge in rock engineering has significantly evolved in recent decades. However, numerous challenges and unanswered questions persist, requiring in-depth investigation through modern theoretical approaches that form the basis of advanced numerical methods. From this perspective, the doctoral thesis aligns with the ongoing need for knowledge development and constitutes a sustained effort to make significant contributions to the field of rock mechanics.

In this context, the thesis addresses complex issues in rock mechanics related to the modeling, simulation, and analysis of the mechanical properties of lignite through specialized software programs based on the Finite Element Method (FEM) and the Discrete Finite Element Method (FDEM).

The Discrete Finite Element Method (FDEM or DEM-FEM) represents an advanced numerical approach used to simulate the behavior of systems composed of discrete and continuous materials. This method combines two analysis techniques: the Finite Element Method (FEM) and the Discrete Element Method (DEM), allowing for detailed modeling of interactions between discrete particles and continuous media.

FDEM serves as a powerful tool for researchers and engineers seeking to study and understand the behavior of discrete materials and their interactions with continuous media. This method is valuable in solving complex and interdisciplinary problems across various fields.

The Discrete Finite Element Method is employed in a wide range of applications, including geotechnics (terrain studies, landslides), civil engineering (foundation analysis, soil behavior), mining industry (rock and mineral behavior), medicine (bone fracture simulation), and many others.

Within the FDEM framework, discrete materials are represented as individual particles or discrete elements. These particles can represent solid objects, granular particles, or other components. Continuous elements represent continuous materials such as solids or fluids and are modeled using the Finite Element Method (FEM). FEM is used to describe the behavior of materials in a continuous medium. FDEM allows for a detailed simulation of interactions between discrete particles and continuous elements, including collisions, contacts, friction, and other complex phenomena.

FDEM simulations are computationally intensive because they require tracking the individual movements of discrete particles. The efficiency and accuracy of simulations must be balanced, and the computation time can be significant depending on the complexity of the system.

To perform FDEM simulations, researchers and engineers utilize specialized software that provides tools for configuration, simulation, and analysis of results. Some software programs include the capability to combine FDEM with FEM to model complex interactions.

Geomechanical analysis of rocks using the Discrete Finite Element Method (FDEM) involves using this numerical technique to model rock behavior in various scenarios and conditions. FDEM allows for a detailed simulation of interactions between discrete particles and continuous elements. This is a numerical approach aimed at understanding the response of rocks to external forces, including natural loads (such as the weight of overlying rocks) and those induced by human activities (such as excavations, constructions, etc.).

Utilizing the Discrete Finite Element Method for geomechanical analysis of rocks can provide a deeper understanding of their behavior under different conditions and loads, proving particularly useful in various fields such as construction, mining, geotechnical engineering, or environmental protection.

In this context, specialized software called IRAZU 2D from the Canadian company GEOMECHANICA, implementing the Discrete Finite Element Method, was used for modeling and simulating the strength characteristics of lignite. The first step in determining the geomechanical behavior of lignite using FDEM was creating the model. This model needed to include rock geometry, material properties, boundary conditions, and other relevant factors.

For conducting FDEM simulations, it was necessary to define the mechanical properties of rocks, such as tensile strength, elasticity modulus, Poisson's ratio, volumetric density, and internal friction coefficient. These properties influence how rocks behave in the simulation.

Initial conditions of the system, such as the initial positions and velocities of discrete elements, were introduced. Boundary conditions were also set to specify how the system interacts with the external environment (e.g., fixed devices or applied loads). By running simulations using FDEM, cracks, sliding, and other geomechanical phenomena could be observed, as well as how rocks interact under loads in specified conditions.

The doctoral thesis is structured into six chapters, subdivided into sub-chapters according to the internal logic and hierarchy of the addressed issues.

Chapter 1, titled "THEORETICAL CONCEPTS RELATED TO THE EXPLOITATION OF MINERAL DEPOSITS THROUGH DAILY WORKS " provides a synthesis of theoretical aspects regarding contemporary mining operations. The open-pit mining of mineral deposits is a complex activity involving the extraction of mineral resources from underground through operations conducted on the Earth's surface. This method of exploitation is applied when deposits are relatively shallow and do not require underground excavations. The extraction process requires attention to detail, careful planning, and responsible resource management. Understanding both theoretical and practical aspects is crucial to ensuring efficient and sustainable exploitation of these resources.

Chapter 2, titled "THEORETICAL CONCEPTS RELATED TO ROCK PROPERTIES AND MECHANICS," highlights the significance of rock properties and mechanics in the field of mining engineering, as they influence rock behavior under various mining conditions, with significant implications for mining project design. These theoretical concepts provide a foundation for understanding the properties and behavior of rocks in different geological and engineering contexts. It emphasizes that understanding rock properties and mechanics is essential for assessing geotechnical risks, designing efficient structures, and exploring/exploiting natural resources such as minerals and fossil fuels.

Chapter 3, titled "DISCRETE FINITE ELEMENT METHOD," details the fundamental theoretical principles underlying this numerical simulation method. It emphasizes that this method is a numerical technique used to simulate the behavior of discrete particles in their surrounding environment. This method finds applications in various fields, including granular mechanics, geotechnics, materials science, geomechanics, and mining engineering. The Discrete Finite Element Method has become essential in research and development, being used in a wide range of domains to understand and design systems involving discrete particles. Additionally, this chapter presents elements related to the use of the Irazu application, designed for simulating various requests in the field of geomechanics based on the principles of the discrete finite element theory.

The simulation of uniaxial compressive strength tests is addressed in Chapter 4, titled "SIMULATING COMPRESSIVE STRENGTH TESTS WITH NO LATERAL UCS CONSTRAINT ON LIGNITE USING DISCRETE FINITE ELEMENT METHOD." To conduct this simulation, a model was created in the SOLIDWORKS application, consisting of a specimen and two compression plates. SOLIDWORKS was chosen for modeling due to its user-friendly drawing environment compared to Irazu. The model was then imported into the Irazu application, where the component parts were identified, and material properties were assigned. Subsequent simulation steps involved setting boundary conditions, with the upper plate fixed, and the lower plate moving upward at a constant velocity, resembling the press model in the Rock Mechanics Laboratory at the University of Petroșani. Before performing simulation calculations, the number of integration steps, integration step size, and the number of steps for graphic information update were established. Post-calculation, the results obtained were presented through both the Irazu and ParaView applications. Additionally, a Python script was implemented in ParaView, allowing direct calculation of parameters based on the integration time step and saving results in an Excel-compatible file.

Chapter 5, titled "SIMULATION OF TENSILE STRENGTH TESTS ON LIGNITE USING DISCRETE FINITE ELEMENT METHOD," involves simulations of indirect tensile

(Brazilian test) and direct tensile strength tests. For direct tensile simulation, two distinct situations were considered: a theoretical simulation where the virtual specimen's ends move in opposite directions, subjecting it to theoretical tensile forces, and a laboratory-type simulation where the specimen is laterally clamped by two gripping devices moving in opposite directions. Similar to uniaxial compression simulation, models for these tests were constructed in SOLIDWORKS, with assigned material properties, and boundary conditions and calculation parameters were set. The results were presented through both Irazu and ParaView applications.

In Chapter 6 of the Thesis, titled "SIMULATION OF SHEAR STRENGTH TESTS ON LIGNITE USING DISCRETE FINITE ELEMENT METHOD," the simulation of lignite shear strength tests is addressed. The chapter begins with theoretical elements related to the determination of shear strength using a predefined failure plane. Since the virtual model subjected to simulation in Irazu aligns with the physical model used in the Rock Mechanics Laboratory at the University of Petroșani, a kinematics study of the shear test was first conducted in SOLIDWORKS. The relationship between the lower plate lifting speed and the upper plate translation speed was determined for various incline angles. Similar to previous simulations, the virtual model for shear strength tests was created in SOLIDWORKS, consisting of the virtual specimen and the two compression plates. Material characteristics, boundary conditions, and calculation parameters were established, and post-calculation results were presented and analyzed through both the Irazu and ParaView applications.

The simulations conducted constituted complex and computationally intensive processes, providing valuable insights into the behavior of this type of rock through the simulation of the aforementioned tests. Simulating the behavior of lignite under uniaxial compression, indirect and direct tensile loading, as well as shear, initially involved creating virtual models consisting of cylindrical or hourglass-shaped specimens and compression plates or gripping clamps.

After importing these models into the Irazu application, the components of each model were identified, and the material characteristics for each component were established. Special attention was given to the properties of the specimens, where mechanical properties of lignite, such as elasticity modulus, Poisson's ratio, and tensile strength, represented average experimental values determined in the laboratory. These values were obtained from experimental data to ensure realistic simulation.

Through the simulations, the behavior of lignite specimens under load was tracked, starting from the initial stages of deformation to failure, detecting the moment when the first cracks appeared between particles and following their evolution until rupture.

Upon completing the simulations, the results were analyzed to obtain information about the uniaxial compressive strength, tensile strength, and shear strength of lignite. This included determining the maximum effort reached during the simulation and assessing the fracture behavior of lignite.

The simulation results were compared with experimental data determined in the laboratory, revealing a very good agreement between simulation and reality.