

Energy Extraction and Processing Science

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With an increasingly tight supply of world energy resources, unconventional oil and gas resources, including shale oil and gas, coal-bed gas, tight sandstone oil and gas, have attracted much attention. Exploration practice in North America shows that among unconventional oil and gas, shale gas has great development potential. The micro mechanisms of fluid occurrence, adsorption, and desorption in micro and nano porous media are important research topics. The production of shale gas needs to focus on the desorption–adsorption process. In general, experimental techniques such as Focus Ion Beam Scanning Electron Microscopy (FIB-SEM) and Transmission Electron Microscopy (TEM) can be adopted to obtain high-resolution micro/nano pore images of shale. On this basis, a numerical model can be constructed. In addition, the corresponding constitutive equations, the gas equation of a state and the multiphase fluid-flow equation are used to carry out the research on various production, transportation and replacement mechanisms of shale gas under numerical simulation. At the same time, it is noted that the occurrence mode of shale gas is classified into free gas, adsorbed gas and dissolved gas. The proportion of adsorbed gas in shale gas varies dramatically from shale-gas reservoir to shale-gas reservoir, generally between 40% and 85%. In addition, the existence of the adsorbed state will also improve the storage capacity of shale gas. Therefore, the occurrence mode of the adsorbed state is considered a critical factor for the successful exploration and development of shale gas. It is necessary to study the relationship between the abundance, maturity, temperature, humidity, and adsorption capacity of shale in shale reservoirs. It can also be noticed that not only is the recovery efficiency of shale oil and gas related to its mode of occurrence, but also, the development of auxiliary additives is an idea to improve the recovery of shale oil and gas [1].

Hot dry rock is a storage form of deep geothermal energy, with rich reserves, and renewable, green and pollution-free characteristics [2,3]. Some developed countries around the world have conducted experiments and commercial operations on hot dry rock geothermal power generation. Fracking and CO₂ fracturing in an enhanced geothermal system are important technical means of developing hot dry rock geothermal energy. Fracking in the development of hot dry rock resources can significantly enhance the permeability and heat production capacity of the reservoir [4]. Usually, the existing hot dry rock geothermal engineering is numerically simulated to study the rock strata movement, rock mechanical behavior and to engineer earthquakes related to heat extraction efficiency and safe mining. During this process, attention is paid to the complex conditions of the deep environment, including high temperature, high stress, high permeability, and the coexistence of multiple states (solid, liquid, gas) [5]. In fact, it is the study on solid–fluid thermal coupling and its engineering response mechanism. The main purpose of the study is to seek effective measures for reservoir transformation and efficient development technology solutions, focus on the formation process of the fractured-rock-mass fracture network, permeability changes,



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heat transfer coefficient, thermal conductivity and other parameter changes, and combine the multi-field coupling theory to establish geothermal-development life prediction and effective technical solutions. Jin et al. [6] conducted two different types of thermal cycling treatments on granite, and analyzed and compared its physical, mechanical, and transport properties after different thermal cycling treatments. Feng et al. [7,8] made experimental research on the fracture mechanics of sandstone after heat treatment at different temperatures. Hu et al. [9] carried out thermal damage tests on granite at different temperatures and quenching cycles, preliminarily revealing the damage mechanism and heat-transfer law of the quenching cycle effect on thermally dried rocks. Hu et al. [10] analyzed the influence of thermal shock fatigue on the physical and mechanical properties and heat conduction of limestone. Apart from that, due to the obvious layered characteristics of shale, it is also necessary to study the relationship between the layered characteristics of shale and its physical and mechanical properties [11,12].

Oil, natural gas, and other energy sources are important material foundations that continuously promote the progress of human society, and belong to traditional energy sources. The extraction technology of oil and natural gas is constantly developing. However, unremitting efforts are required to carry out research on efficient and environmentally friendly extraction technology innovation. Marsden et al. [13] indicated some promising potential applications of nanotechnology in coalbed methane fracking. How to realize the dynamic equilibrium of energy exploitation and environmental protection is a challenge to be solved urgently. For example, issues caused by energy exploitation such as water pollution, air pollution, and vegetation damage are becoming increasingly prominent and require in-depth research. The above is an overview of the macro level of mining technology and the comprehensive factors of environmental protection.

At the micro level, the simulation of energy molecules and their movement, transportation, and changes in the mining environment are of great importance, and they are related to the efficient extraction and utilization of energy. It is necessary to study the theory and model construction of energy molecules, molecular physical and chemical reactions under multiphysics simulation, and molecular dynamics. Beyond that, it is worth noting that cement slurry, waxy crude oil, drilling fluid and water solvent in petroleum engineering are all non-Newtonian fluid, and the research on their flow phenomena is a difficulty for scientific researchers. At present, no universally applicable non-Newtonian-fluid constitutive procedure has been found. In the some of the research areas outlined above, researchers are currently conducting in-depth analysis. For example, carbonate rock has been used as a reservoir of oil and gas. Zhang et al. [14] studied the interaction of carbonate fluid by heating carbonate mineral and rocks with four different acid solutions (saturated CO_2 and H_2S solution, HCl , CH_3COOH) in a sealed sample chamber. In fractured carbonate rock, the reservoir quality is controlled by fracture properties [15]. Coal is composed of complex aggregates. The characterization of the coal molecular structure directly affects the evaluation of the coal reservoir and the enrichment mechanism of coalbed methane. Considering this, the macromolecular structure of different ranks of coals should be studied in detail, and a model should also be built. The study of this numerical simulation molecular model is conducive to the basic research on the chemical structure of coal and that on coal pyrolysis and biogas conversion technology. Other than that, the underground gasification of coal is an effective development technology solution to in situ coal mining and utilization, and involves coal molecular pyrolysis and molecular movement issues in the mechanical and chemical environment of mines. Using the numerical simulation of coal pyrolysis molecules and their chemical-reaction relationship with oxygen, as well as the decomposition and recombination process of molecules, is an important technical exploration for the production of underground coal gasification. At the same time, its molecular movement under pyrolysis has an impact on the surrounding rock, and the resulting rock mechanical problems, including the instability of the rock-strata movement, rock-fracture failure and changes in the formation water environment, have a very huge impact. In this case, it is of great necessity to conduct large-scale simulation research on

the coal pyrolysis process in different atmospheres using molecular-dynamics simulation methods, and analyze the chemical reactions and carbon structure changes therein. Before conducting numerical simulations, the mineral composition should be accurately studied. For example, coal is broken and dissociated, and the dissociation laws of its chitin, vitrinite, and inertinite at different particle sizes are studied. Based on this, density gradient centrifugation is adopted to study the separation of macerals, and further research is performed on the impact of ultrasound assistance on the separation effect.

Some scholars have conducted research on the relevant research directions mentioned above. For example, well-developed pores and fractures in coal reservoirs are the main locations for storage and migration [16]. The characteristics of pore and fracture structures in coal and their evolution during mining are crucial for preventing gas outburst and improving gas extraction efficiency [17]. In terms of related studies, Ajayi et al. [18] utilized a research model from the National Institute of Occupational Safety and Health (NIOSH) in the United States to study the effects of geological conditions, crack length, and leaked-gas properties on underground transportation. The results indicate that the prediction of the underground gas flow decreasing with the increase in crack length is specifically targeted at non-gas-bearing formations. Zhang et al. [19] reconstructed the micro fracturing structure of coal in the Surat Basin by employing the 3D shape measurement system and the stitching algorithm, then generated transparent models characterizing the fracturing structure using microfluids, and measured water invasion in the micro fracture model under different conditions through visual experiments. Abaimov et al. [20] developed an experimental device based on the characteristics of underground coal-gasification engineering, and studied the characteristics and advantages of a self-heating single-set atmospheric-pressure bituminous-coal fluidized-bed air-blown gasifier. Zhang et al. [21] conducted a cyclic triaxial loading and unloading (CTLU) experimental study on the acoustic emission monitoring of deep coal samples. Adsul et al. [22] used FTIR and Raman spectroscopy to comprehensively investigate the microstructure of low- to medium-rank tertiary coal in Megarava, as well as the effect of the control mechanism of its microstructure on its hydrocarbon potential. Mishra et al. [23] adopted homogeneous and shrinking-core kinetic models to calculate the results of coal gasification and verify the accuracy of the model. Wang et al. [24] adopted the computational fluid-dynamics software Fluent to simulate the influence of various parameters on the pressure evolution of specific parts of the pipeline for filling mining. Krishnamorthy [25] followed computational fluid dynamics, with add-on ash deposition and shelving models employed, to predict outer-ash deposition and shelving rates during the co-commerce of coal/RH in AIR and O₂/CO₂ optimizer composites. Nesbitt et al. [26] introduced an automatic classification method for microstructure blocks which can be used to classify small classifications of coke microstructure blocks (approximately 450 μm³) from 3D computed tomography scans. Uznetsov et al. [27] studied the chemical composition, structure, and plastic properties of different grades of coal in Mongolian deposits. Kossovich et al. [28] combined various Nanoindentation and Raman spectroscopy techniques to investigate the mechanical behavior of the selected coal by increasing the cyclic nano indentation with a peak load and quasi-static load. In the future, energy extraction will increasingly develop towards deep strata, and finding solutions will require overcoming greater challenges. As the most prominent environment at great depths is the temperature and geostress environment, especially the various high-temperature environments [29–31], there are significant changes in the mechanical properties of deep rock layers with engineering disturbances, and the stability of surrounding rocks is pronounced.

Based on the above analysis, we believe that conducting research on this topic is required. The theme we are launching will be specifically centered on the concept of new energy-security mining technology and sustainable development, such as protecting the environment from potential project damage and ensuring internal mechanisms for sustainable energy utilization. The research includes but is not limited to the following aspects:

- The monitoring and control of dust in energy extraction processes;
- Macromolecular modeling of different types of energy sources;

- CO₂ sequestration/hydrogen storage in geological formations;
- Environmental protection in resource development;
- The application of computer science to solve safety problems in energy extraction;
- The characterization of size, shape, surface area, pore structure, and strength of energy particles and agglomerates (including the sources and effects of interparticle forces);
- The adsorption of auxiliary agents at energy interfaces or surfaces;
- The adsorption process generating competitive behavior;
- Mathematical modeling and numerical simulation of coupled processes;
- The creation, storage, and transport of unconventional energy sources;
- The prevention of and reduction in geological hazards in mines;
- The mathematical aspects of rock mechanics and rock engineering;
- The production and storage of geological energy.

We encourage further research and strongly appeal for the publication of relevant research results concerning this topic we are focusing on. These studies will enrich energy-extraction and -process science, reflect the latest developments and directions in the research field, and enable the timely and rapid dissemination of research conclusions and viewpoints, promoting the development of the discipline and the formation of new research ideas in the future.

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