

Article

Study on the Sealing Capability of Overlying Mudstone of Coal Under Thermal Action During Underground Coal Gasification

Chunlin Jiao ^{1,2}, Xinyang Yao ^{1,2}, Xin Li ^{1,2,*} , Wanli Leng ^{1,2}, Shuxun Sang ^{1,2,*}  and Zhenpeng Hu ³

¹ School of Geology and Mining Engineering, Xinjiang University, Urumqi 830047, China; jiao2630328@163.com (C.J.); yaoxinyang0920@163.com (X.Y.); wanlileng@163.com (W.L.)

² Xinjiang Key Laboratory for Geodynamic Processes and Metallogenic Prognosis of the Central Asian Orogenic Belt, Xinjiang University, Urumqi 830017, China

³ Xinjiang Key Laboratory of Coalbed Methane Exploration and Development, Urumqi 830009, China

* Correspondence: lixinwaxj@xju.edu.cn (X.L.); shxsang@cumt.edu.cn (S.S.)

Abstract

This study systematically investigates the microstructure, physical properties, and sealing capacity of mudstone under thermal action using scanning electron microscopy (SEM), high-pressure mercury intrusion, breakthrough pressure testing, and diffusion coefficient analysis. Pore-throat structure, porosity, permeability, breakthrough pressure, and diffusion coefficient were measured at 25, 300, 600, 900, and 1200 °C, while additional SEM observations were conducted at 100, 200, 400, and 500 °C. Based on the integration of these discrete measurements and supplementary SEM observations, the evolution of mudstone sealing capability was interpreted as follows. (1) At 25–200 °C, mineral dehydration exposes primary pores, with porosity and permeability increasing gradually while strong sealing capacity is maintained. (2) At 200–400 °C, clay mineral dehydration, thermal expansion, and secondary fracture development increase pore connectivity, resulting in a sharp decline in sealing capability. (3) At 400–1200 °C, mineral structure collapse, pore-fracture connection, and mineral melting further increase porosity and permeability, leading to progressive sealing failure. (4) The threshold temperature for mudstone sealing failure is inferred to be approximately 400 °C. (5) Mudstone affected by temperatures below 200 °C is recommended as an effective caprock for underground coal gasification chambers. This study provides theoretical guidance for caprock selection and safe operation in underground coal gasification engineering.

Keywords: underground coal gasification; sealing capability; caprock; mudstone; thermal action



Academic Editor: Alessandro Cosenza

Received: 5 July 2026

Revised: 21 July 2026

Accepted: 23 July 2026

Published: 27 July 2026

Copyright: © 2026 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article distributed under the terms and

conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

1. Introduction

Underground coal gasification (UCG) technology significantly enhances resource utilization efficiency, mitigates safety and ecological risks associated with conventional mining operations, and may reduce some environmental impacts of conventional mining under controlled conditions [1–3]. Compared to conventional mining methods, the high-temperature fields generated during underground coal gasification (UCG) alter the physicochemical properties, mechanical behavior, and sealing integrity of surrounding strata in gasification chambers [4–6]. This leads to a sharp decline in thermal stability and sealing capacity of the rock layers, and even triggers instability and collapse, severely compromising the effectiveness of UCG operations. Therefore, the thermal stability and

sealing integrity of key caprock layers under thermal effects are critical to the efficient and safe operation of gasification chambers, making their investigation imperative.

The thermal-physical properties of mudstone under high-temperature conditions are intrinsically linked to its internal microstructure, encompassing differential thermal expansion of constituent minerals upon heating and stress-induced microstructural rearrangement [7–10]. After thermal treatment at different temperatures, distinct microstructural variations are observed in mudstone: interlayer detachment and intralayer fractures emerge at 130 °C and 150 °C [11], while under high temperatures of 400–500 °C, the porosity of mudstone increases significantly, compromising the sealing capacity of mudstone caprock [12,13]. Under high-temperature conditions, the overall structural performance of mudstone deteriorates, with approximately 400 °C identified as the threshold temperature for mudstone damage under cyclic thermal stress; high-temperature exposure significantly alters the physical sealing characteristics of caprock mudstone [14]. It can be concluded that thermal effects significantly alter the physical sealing properties of rocks, thereby compromising the sealing capacity of caprock sealing systems. In underground coal gasification (UCG), the thermal influence within the roof strata extends up to approximately 15 m. Regions within 0–10 m of the gasification chamber experience severe high-temperature effects, whereas beyond 10 m the temperature decreases to approximately 200 °C [15–19].

International studies have also investigated the coupled thermal and geomechanical evolution around UCG reaction channels. Coupled thermo-mechanical simulations have revealed that heat propagation around the gasification cavity alters the stress, deformation, and permeability of the surrounding strata [20,21]. Numerical studies of carbonaceous material conversion in coal-seam channels have shown that heat transfer, fluid flow, and species transport produce a strongly nonuniform temperature field [22]. Thermo-hydraulic-chemical modeling further demonstrates that temperature development, pore-structure alteration, and solid–gas conversion jointly control the progressive growth of the gasified cavity [23]. Laboratory UCG studies also indicate that temperature evolution in the immediate roof is closely associated with rock-strength degradation and cavity formation [24]. These findings highlight the need to evaluate caprock integrity by considering thermal exposure together with pore-fracture evolution, mechanical degradation, and cavity development.

However, the temperature-dependent sealing behavior of mudstone caprocks in the Baikouquan area remains insufficiently understood. Previous studies have not jointly characterized thermally induced microstructural and pore-throat changes, quantified sealing performance through breakthrough pressure and gas diffusion tests, or linked these experimental results to the temperature distribution around UCG chambers. Consequently, the thermal evolution stages, critical temperature, and controlling mechanisms of mudstone sealing capacity in this area remain unclear.

This study focuses on mudstone from the Xishanyao Formation in the Baikouquan area, conducting scanning electron microscopy (SEM) and high-pressure mercury intrusion experiments to investigate microstructural morphology and pore-throat characteristics of caprock mudstone under varying temperatures. Conventional physical property tests are performed to analyze porosity and permeability evolution. Sealing parameters, including breakthrough pressure and diffusion coefficient, are measured to evaluate sealing capacity variations. By integrating microstructure physical properties sealing capacity analyses and incorporating stratigraphic conditions and temperature distribution patterns, this research delineates sealing characteristics and controlling factors of caprock mudstone across different thermal stages. Ultimately, it establishes sealing mechanisms of mudstone caprocks during underground coal gasification (UCG), providing theoretical foundations for selecting effective sealing caprocks in UCG engineering.

2. Methods

2.1. Geological Background

The study area is located in the Baikouquan region at the northwestern margin of the Junggar Basin, Xinjiang, China (Figure 1a), specifically within the central segment of the Karamay–Baikouquan thrust-nappe tectonic belt in the Ke-Bai fault zone (Figure 1b) [25,26].

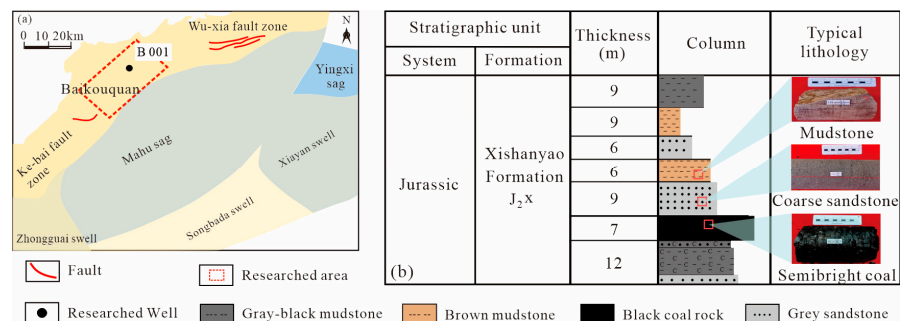


Figure 1. Column diagram of coal measure strata of a well in Baikouquan area.

The Jurassic Xishanyao Formation gasification coal seam has a thickness of 6–8 m, classified as long-flame coal with medium-low ash content, high volatile matter, abundant vitrinite, and minor liptinite and inertinite. The coal seam is directly overlain by coarse-grained sandstone with well-developed pores and a loose, friable structure. Above the sandstone is a regionally continuous purplish-brown mudstone unit with a dense texture and a single-layer thickness of 5–7 m. Owing to its lithological characteristics, thickness, and stratigraphic position, this mudstone was selected as the potential caprock and the primary research subject in this study.

2.2. Experimental Procedure

This study aims to perform an integrated analysis of the sealing capability of overlying mudstone under thermal effects during UCG. The experimental methods encompass sample collection and preparation, thermal treatment, microstructural analysis, pore-structure characterization, and sealing capability testing. The detailed experimental procedure is depicted in Figure 2.

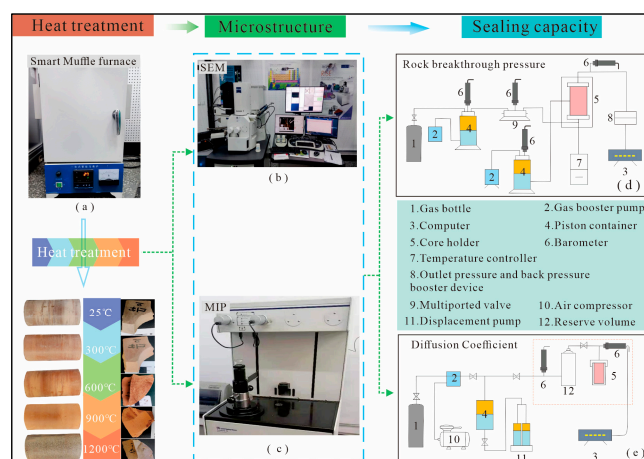


Figure 2. Test process and corresponding instruments. (a) heat-treatment equipment and rock specimens treated at different temperatures; (b) scanning electron microscope used for microstructural characterization; (c) mercury intrusion porosimeter used for pore-structure characterization; (d) experimental system for measuring rock breakthrough pressure; and (e) experimental system for determining the gas diffusion coefficient.

2.3. Rock Sample Collection and Preparation

The caprock mudstone samples were collected from the Baikouquan area at a burial depth of approximately 810–812 m. Preserved in sealed plastic wrap, the samples were transported to and stored in a constant temperature/humidity laboratory environment. Core plugs ($\phi 25 \text{ mm} \times 50 \text{ mm}$) were drilled perpendicular to the bedding planes for physical property and sealing capability tests. All specimens used in the different test groups were obtained from the same core column and prepared with the same orientation to minimize variations caused by lithological heterogeneity and anisotropy. The specimens exhibit a purplish-brown color in their natural state, with an average density of 2.29 g/cm^3 .

2.4. Experimental Scheme

Before thermal treatment, the specimens were maintained in their natural state without additional drying. Thermal treatment was conducted in a programmable muffle furnace (SRJX-4-13A, Figure 2a) under an air atmosphere. For each of the five principal temperature conditions (25, 300, 600, 900, and 1200°C), one specimen was used for each test item, including porosity, permeability, high-pressure mercury intrusion, SEM observation, breakthrough pressure, and diffusion coefficient measurement. One additional specimen was prepared for SEM observations at 100, 200, 400, and 500°C to characterize the intermediate microstructural evolution. The specimens were heated to the target temperatures at a rate of 5°C/min and held for 4 h [27,28]. After thermal treatment, the furnace was switched off, and the specimens were allowed to cool naturally to room temperature inside the closed furnace.

Scanning electron microscopy (SEM) analysis was performed using a Zeiss Sigma 300 instrument (Figure 2b). The integrated console was utilized to adjust the operating voltage to 3 kV, set micrometer-level magnification, and fine-tune image focus until optimal clarity was achieved. At each temperature, one specimen was examined by SEM. Multiple fields of view were observed on the specimen, and the image presented in the manuscript was selected to represent the microstructural features repeatedly observed within that specimen. Additional SEM observations at 100, 200, 400, and 500°C were used to supplement the characterization of intermediate microstructural evolution.

High-pressure mercury intrusion (HPMI) experiments were conducted using a Micromeritics AutoPore V instrument (Figure 2c), with the maximum mercury intrusion pressure set to 413 MPa. Pore-structure parameters, including pore volume, average pore diameter, and pore size distribution, were derived from automatically recorded mercury intrusion-extrusion data combined with the Washburn equation [29].

Breakthrough pressure of the mudstone was determined following the petroleum industry standard <Determination Method of Gas Breakthrough Pressure in Rock> [30]. Given the high clay mineral content of the mudstone, kerosene was selected as the wetting fluid. A net confining pressure of 22 MPa was applied and maintained throughout the experiment to ensure equivalence with the effective overburden pressure, enabling direct measurement of the mudstone sealing capacity (Figure 2d).

The nitrogen diffusion coefficient was measured under constant-temperature and constant-volume conditions. The test temperature was maintained at 40°C . The amount of nitrogen diffusing into the specimen was calculated from the recorded pressure variation using the real-gas equation of state, $PV = ZnRT$, and mass conservation. Based on one-dimensional Fickian diffusion, the nitrogen uptake at time t can be expressed as:

$$n_t = 2AC_0\sqrt{\frac{Dt}{\pi}} = k\sqrt{t} \quad (1)$$

And the diffusion coefficient was calculated as:

$$D = \frac{k^2 \pi}{4A^2 C_0^2} \quad (2)$$

where n_t is the amount of nitrogen diffused into the specimen at time t (mol), A is the effective diffusion area (m^2), C_0 is the nitrogen concentration at the open boundary ($\text{mol} \cdot \text{m}^{-3}$), t is the diffusion time (s), and k is the slope of the linear relationship between n_t and $\sqrt{t}$ ($\text{mol} \cdot \text{s}^{-1/2}$). The calculated diffusion coefficient D is expressed in $\text{m}^2 \cdot \text{s}^{-1}$.

3. Results

3.1. Apparent Morphological Changes of Overlying Mudstone Samples Under Thermal Action

In Figure 3, the apparent morphology of the mudstone has changed significantly after being treated at different temperatures. As the temperature rises to 300 °C, the mudstone gradually transforms from purplish-brown to reddish-brown, with the color gradually deepening. As the temperature rises to 600 °C, the color deepens to a brick red, and the layering surface becomes clearly visible. When the temperature reaches 900 °C, the mudstone sample becomes noticeably lighter and exhibits a pale pinkish-brown color, accompanied by the development of fine surface cracks. When the temperature reaches 1200 °C, the mudstone becomes dark brown, and microscopic holes appear on the sample surface. The rock column exhibits pronounced collapse-like deformation, which may be associated with high-temperature softening, and some specimens disintegrate along the bedding planes.

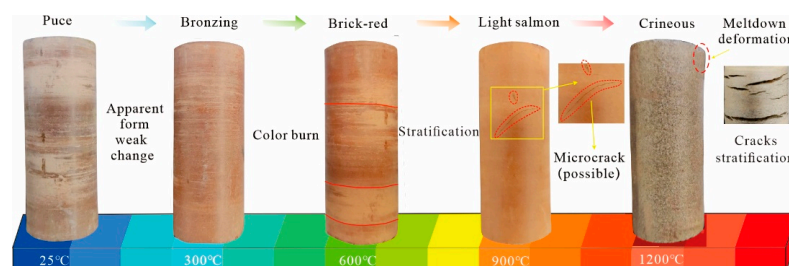


Figure 3. Apparent morphology of caprock after heat treatment.

3.2. Changes in Microscopic Pore Structure Under Thermal Action

The microstructure of overlying mudstone at different temperatures was observed via SEM to understand the morphological characteristics of pores and fractures. As shown in Figure 4, there are some primary pores (microcracks) in the caprock at ambient temperature. As the temperature is raised to 200 °C, the primary pores in the sample gradually expand during the experiment, and the structural and morphological changes are not significant (Figure 4a–c). When the temperature rises to 300 °C, the primary pores expand once again and are accompanied by the generation of new pore fractures. The scale of the new fractures is relatively small (Figure 4d). At 400 °C, some primary pores appear locally closed, which may be associated with the thermal expansion of mineral grains (Figure 4e). At 400 °C, due to the thermal expansion of minerals, the primary pores present a closed state (Figure 4e). When the temperature rises to 500 °C, the pores expand again, possibly owing to thermally induced cracking, and the morphology of the primary fractures begins to change (Figure 4f). When the temperature rises to 600 °C, the primary pore fractures further increase, the newly developed thermally induced fractures expand further, and non-cohesive cracks appear between adjacent mineral grains (Figure 4g). As the temperature reaches 900 °C, the newly formed fractures and cavities further expand. Changes in the morphology of mineral and cementing-material boundaries become evident, including local boundary

recession and irregular fractures. These features may reflect high-temperature softening or partial melting of cementing phases. Pronounced structural changes and transgranular cracks are also observed in some mineral grains (Figure 4h). When the temperature rises to 1200 °C, recession along mineral boundaries becomes more pronounced. Small pores become interconnected, and the pore size increases further. Granular deposits are also observed on the sample surface, which may be related to salt crystallization during cooling (Figure 4i).

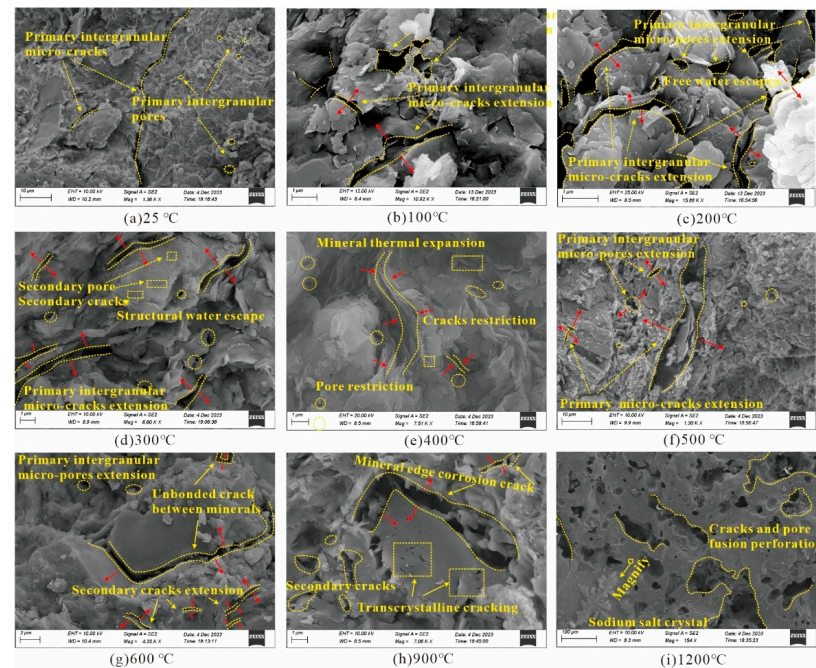


Figure 4. Micromorphological characteristics of the mudstone caprock at different temperatures.

3.3. Characteristics of Pore-Throat Structure and Main Seepage Channels

The pore-throat radius of mudstone exhibits a pattern of initial increase, subsequent decrease, and final increase with rising temperature. From 25 °C to 600 °C, pore-throat radii expand sharply: the maximum radius grows from 50 nm to micrometer-scale, while the average radius only doubles. Displacement pressure drops abruptly at 300 °C. At 900 °C, the maximum pore-throat radius shows a declining trend, with the average radius reduced to half of its 600 °C value and displacement pressure tripled. By 1200 °C, the maximum pore-throat radius expands to 10 µm-scale, the average radius increases tenfold, and both displacement pressure and median radius decrease. At 600 °C, pore-throat size distribution becomes uniform with improved sorting, and the mudstone exhibits a coarse skewness (Table 1).

Table 1. Quantitative characteristics of pore permeability and capillary pressure curves of mudstone.

Temperature/°C	Displacement Pressure/MPa	Median Pressure/MPa	Maximum Pore-Throat Radius/µm	Median Pore-Throat Radius/µm	Mean Pore-Throat Radius/µm	Sorting Coefficient	Maximum Offensive Saturation/%	Mercury Removal Efficiency/%
25	13.072	35.614	0.048	0.018	0.014	9.051	77.485	40.856
300	0.96	19.159	0.65	0.033	0.026	1.495	71.799	40.158
600	0.957	14.501	1.056	0.043	0.029	0.201	90.586	51.548
900	2.891	18.858	0.216	0.033	0.014	1.994	62.283	1.156
1200	0.069	4.923	9.036	0.127	0.131	2.479	68.244	27.408

At 25, 300, and 600 °C, semi-closed pore throats were prevalent, and the mercury withdrawal efficiencies were 40.856%, 40.158%, and 51.548%, respectively. Although some

variation occurred, no pronounced decline was observed before 600 °C. With further temperature increase, partial melting of minerals and cementing materials enlarged the pore cavities, while molten phases blocked some pore throats during cooling. This process generated more isolated and ink-bottle pores and increased mercury entrapment. Consequently, the mercury withdrawal efficiency decreased sharply to 1.156% at 900 °C and then recovered to 27.408% at 1200 °C.

As shown in Figure 5, the flow capacity of mudstone evolves in tandem with pore-throat variations as temperature increases. At 25 °C, pore throats are concentrated in the 0.01–0.03 µm range, with primary microfractures (0.4 µm) forming flow pathways that balance with intrinsic pore networks, creating dual flow channels. Excluding fracture effects, the mudstone exhibits weak flow capacity at this stage. By 300 °C, pore-throat radii expand significantly, and enhanced pore connectivity leads to overlapping peaks of porosity and permeability, dominated by pore-network flow. At 600 °C, thermal expansion induces irreversible structural fracturing, generating microfractures whose connectivity far surpasses intrinsic pore networks, shifting flow dominance to large-scale fracture pathways. At 900 °C, pore-throat radii contract globally, concentrating in the 0.06–0.25 µm range. By 1200 °C, pore-throat radii expand markedly, and interconnected pore-fracture networks establish large-scale flow pathways as the primary conduits.

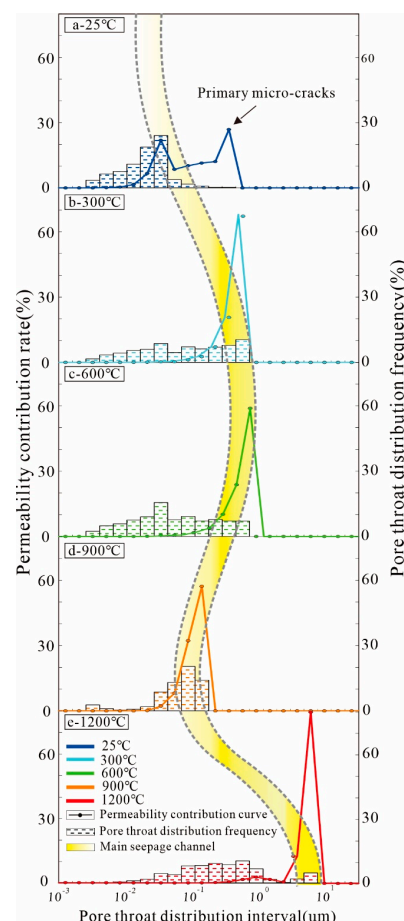


Figure 5. Pore diameter distribution and main seepage channels of mudstone at different temperatures.

3.4. The Changes in Porosity and Permeability Characteristics of Overlying Mudstone Under Thermal Effects

As shown in Figure 6, with the increase in heat treatment temperature, the porosity rises slowly at first (25–900 °C). When the temperature rises to 900 °C, the porosity begins to increase sharply, and at 1200 °C, it rises to 1.69 times that at 900 °C. Permeability increases

gradually from 25 to 600 °C, rises sharply between 600 and 900 °C, reaches its maximum at 900 °C, and then decreases at 1200 °C.

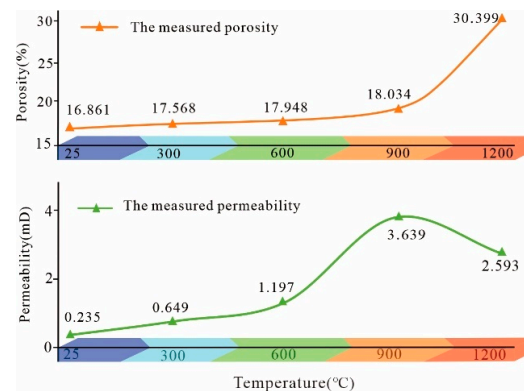


Figure 6. Measured porosity (permeability) variation curve with temperature.

3.5. The Characteristics of Breakthrough Pressure and Diffusion Coefficient of Overlying Mudstone Under Thermal Action

Breakthrough pressure is a characteristic parameter for the evaluation of the sealing capacity of overlying mudstone [31]. The mudstone caprock in the Baikouquan area exhibits dense lithology. At 25 °C, the mudstone remains unbreached, demonstrating excellent sealing integrity. When temperature rises to 300 °C, the breakthrough pressure decreases to approximately 20 MPa. With further temperature elevation, the breakthrough pressure of mudstone samples plummets sharply. Beyond 600 °C, the breakthrough pressure remains around 0.7 MPa, indicating complete loss of sealing capacity (Figure 7). The diffusion coefficient of mudstone exhibits a trend consistent with its measured permeability. From 25 to 600 °C, the diffusion coefficient increases gradually. It then rises sharply between 600 and 900 °C, reaches its maximum at 900 °C, and decreases at 1200 °C (Figure 7).

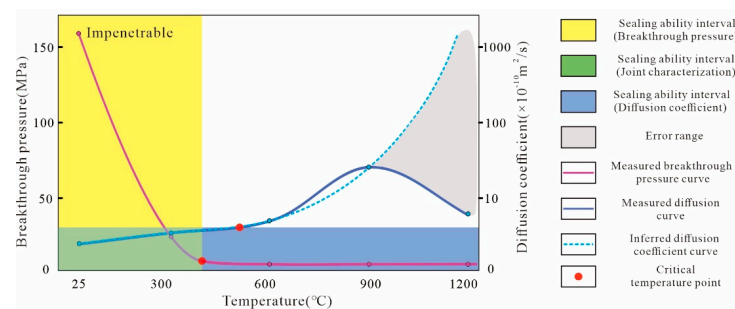


Figure 7. Combined characterization of sealing capacity by diffusion coefficient and breakthrough pressure.

4. Discussion

4.1. Evaluation of Sealing Capability

Previous studies indicate that when pore-throat radii are smaller than 100 nm, breakthrough pressure remains high, typically ensuring robust sealing capacity in caprocks. Conversely, when pore-throat radii exceed 300 nm, breakthrough pressure decreases to a constant value, reflecting insufficient sealing integrity and heightened vulnerability to gas breakthrough [32–34].

The pore-throat radius is inversely proportional to breakthrough pressure, with the latter being predominantly governed by large-scale pore-throat radius. At 25 °C, the maximum pore-throat radius measures 48 nm, and the rock's breakthrough pressure remains unbreachable under testing conditions. At 300 °C, pore throats larger than

300 nm account for 18% of the total, providing dominant pathways for gas breakthrough and causing a sharp decline in breakthrough pressure. By 600 °C, the maximum pore-throat radius increases to 1 µm. Despite 60% of pore throats remaining below 100 nm, large-scale pore throats facilitate efficient gas breakthrough, stabilizing the breakthrough pressure at a constant value and indicating complete loss of caprock sealing capacity. The breakthrough pressure decreases substantially from approximately 20 MPa at 300 °C to approximately 0.7 MPa at 600 °C, indicating pronounced deterioration of the sealing capability within this temperature interval. Meanwhile, SEM observations at 400 °C reveal notable changes in the microstructure of the mudstone. Taken together, the changes in breakthrough pressure and microstructure support the inference of an approximate critical temperature of 400 °C for the thermal deterioration of mudstone sealing capability (Figure 8).

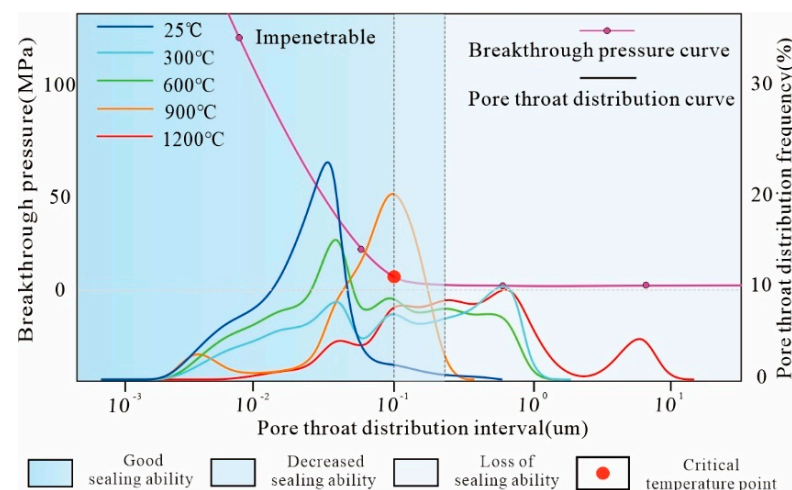


Figure 8. Relationship between pore-throat distribution and breakthrough pressure as a function of temperature.

The gas diffusion coefficient is a critical physical parameter used to assess the diffusion capacity of natural gas [35]. The diffusion coefficient is primarily influenced by temperature and pressure conditions, rock physical properties, and fluid characteristics [36]. Previous investigations have demonstrated that when the pore-throat radius is less than 10 nm, the diffusion coefficient can be as low as 10×10^{-10} – 10×10^{-12} m²/s. At this juncture, gas migration is essentially halted, and the caprock is typically endowed with excellent sealing properties. Generally, the diffusion coefficient value of the caprock is within the range of 10×10^{-10} – 10×10^{-12} m²/s, at which the pore-throat radius is approximately 10 nm–100 nm. The diffusion coefficient value of the non-caprock is approximately 10×10^{-8} – 10×10^{-9} m²/s [37–39].

Permeability and diffusion coefficient both reaching their maximum values at 900 °C and then decreasing at 1200 °C, the pore-throat dimensions increase markedly at 1200 °C, playing a pivotal role in gas diffusion. At 25 °C, excluding fracture-induced flow effects, the dominant pore throats governing permeability are concentrated in the 10–100 nm range. The diffusion coefficient remains at $\sim 1.0 \times 10^{-10}$ m²/s, indicating effective sealing performance. At 300 °C, pore-throat radiation expands to 600 nm, with primary flow pathways shifting markedly rightward. The measured diffusion coefficient increases by 1.4 times compared to 25 °C, falling within the effective range for conventional caprocks, suggesting partial sealing integrity. At 600 °C, the maximum pore-throat radius reaches 1 µm, and the dominant flow pathways continue to shift toward larger pore sizes. The diffusion coefficient rises to 5.874×10^{-10} m²/s, which remains within the range commonly reported for caprocks. However, the breakthrough pressure has already decreased to approximately 0.7 MPa, indicating severe deterioration of the sealing capacity. This contrast implies that the diffusion coefficient alone is insufficient to evaluate caprock performance. In addition,

the elevated gas concentrations and strong thermal gradients that characterize actual UCG environments could further promote gas diffusion, although this possibility remains to be tested by coupled transport simulations or in situ measurements. At 900–1200 °C, measured diffusion coefficients exceed the effective sealing range, leading to complete loss of caprock integrity. The reduced diffusion coefficient at 1200 °C may stem from post-melting pore-throat occlusion caused by mineral phases such as feldspar, quartz, and cementing materials during cooling (Figure 9).

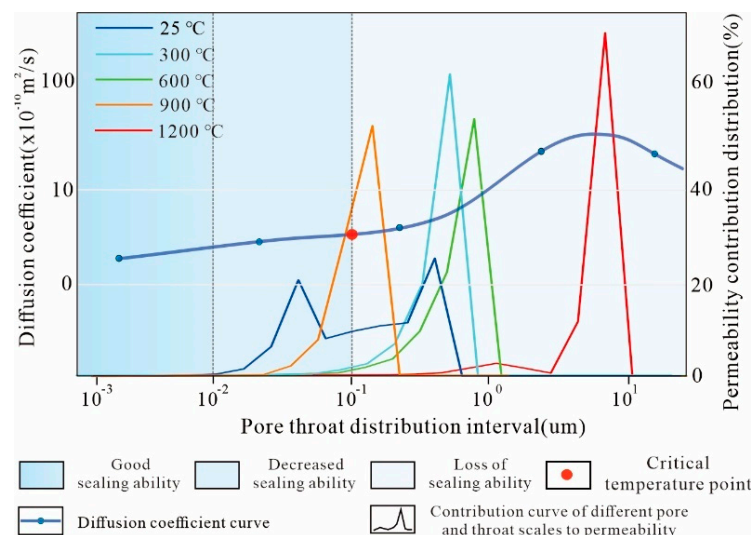


Figure 9. Plot of permeability contribution curves versus diffusion coefficient versus temperature change.

4.2. Stage Segmentation According to Evolutions of Minerals and Pore Structure During Thermal Action

Based on the experimental results presented above, several laws can be concluded. In aspect of microstructural morphology, from 25 °C to 200 °C, the primary manifestation is the exposure of original pores and fractures resulting from the evaporation of free water and interlayer water. Between 200 °C and 400 °C, these pores and fractures undergo micro-expansion or closure due to anisotropic mineral expansion and the loss of structural water. In the range of 400 °C to 600 °C, new microfractures develop between existing fractures and pores as a result of mineral expansion and fragmentation, with further loss of structural water along cleavage planes leading to an increase in pore size. At temperatures from 600 °C to 900 °C, both primary fractures and transgranular cracks continue to expand until they penetrate completely, causing non-adherent cracks to enlarge further. Finally, within the temperature range of 900 °C to 1200 °C, pores and fractures become distinctly visible due to melting processes that facilitate their connectivity.

Regarding pore-throat characteristics, at 25–600 °C, the pore-throat size increases with increasing temperature, while at 600–900 °C, it decreases, and at 900–1200 °C, it increases again. The main permeability pathways remain consistent with the changes in pore-throat size. In terms of physical properties, porosity increases slowly from 25 to 900 °C and then rises sharply at 1200 °C. Permeability increases gradually from 25 to 600 °C, rises sharply to its maximum at 900 °C, and then decreases at 1200 °C. In terms of sealing characteristics, breakthrough pressure decreases sharply with increasing temperature and remains close to 0.7 MPa from 600 to 1200 °C. The approximate critical transition is inferred to occur near 400 °C. The diffusion coefficient increases gradually from 25 to 600 °C, rises sharply to its maximum at 900 °C, and then decreases at 1200 °C.

Based on microstructural morphology, and features of caprock mudstone at varying temperatures, while considering the trends in pore-permeability changes and sealing parameter characteristics, the temperature stages influencing the alterations in sealing capability of caprock mudstone during UCG are categorized as follows: low-temperature stage (25–200 °C), low-to-medium-temperature stage (200–400 °C), medium-temperature stage (400–600 °C), medium-to-high-temperature stage (600–900 °C), and high-temperature stage (900–1200 °C).

4.3. Changes in the Sealing Capability at Different Temperature Stages and Their Control Factors

Low-temperature stage (25–200 °C): The slight expansion and exposure of primary pores may be associated with the release of free water, interlayer water, and adsorbed water from the mudstone matrix (Figure 4a–c). Dominant pore-throat radii are concentrated within 15–25 nm (Figure 5a). At this stage, flow pathways are primarily governed by the mudstone matrix, with poor connectivity between pores. The diffusion coefficient increases gradually, and the mudstone remains unbreached, indicating exceptionally strong sealing capacity. This high-performance caprock, positioned at the uppermost layer, demonstrates superior sealing integrity (Figure 10).

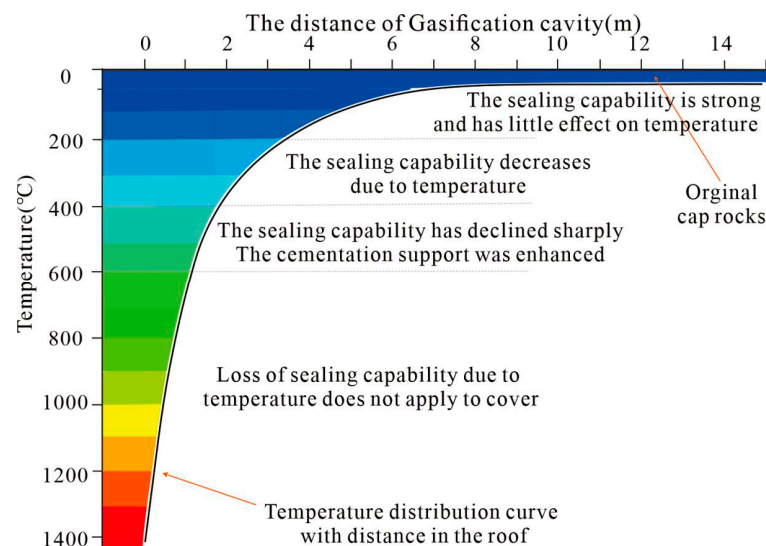


Figure 10. Characteristic diagrams at different temperature levels (Quote from [15]).

Low-to-medium temperature stage (200–400 °C): The development of new intergranular fractures and the expansion of primary fractures may be associated with the loss of crystalline and structural water from clay-rich components (Figure 4d). The pore-throat radii in mudstone increase tenfold, with dominant radii concentrated in the 0.04–0.25 μm range. Flow pathways are dominated by throats of 0.5 μm scale, exhibiting a pronounced rightward shift (Figure 5b). Porosity, permeability, and diffusion coefficient increase progressively. On one hand, thermally induced fragmentation may produce finer particles that infill some small pores; on the other, thermal expansion of mineral grains may induce local contraction of primary intergranular fractures (Figure 4e), thereby slowing permeability growth. At 300 °C, the mudstone is breached, with a breakthrough pressure of approximately 20 MPa, then the breakthrough pressure further decreases to approximately 0.7 MPa at 600 °C (Figures 7 and 8), indicating pronounced deterioration of sealing capability between these two temperatures. Within this interval, the SEM observations at 400 °C reveal notable changes in the mudstone microstructure. Together, these changes support the inference of an approximate critical temperature of 400 °C and indicate weakened caprock sealing capability during this stage (Figure 10).

Medium-temperature stage (400–600 °C): Beyond the approximate critical temperature, clay-rich components may undergo further structural water loss, which can promote structural alteration and the development of transgranular cracks. Dehydration and possible local softening of cementing materials may contribute to the widening of non-cohesive intergranular cracks (Figure 4g) [40,41]. Porosity and permeability show sustained increases. Compared with the 300 °C condition, the pore-throat sizes change only slightly, whereas the pore-throat radius distribution becomes narrower (Figure 5b,c), possibly owing to the redistribution and re-solidification of softened cementing materials during cooling. This process may locally occlude pore throats previously expanded at high temperatures. The dominant flow pathways persist as 0.5 µm-scale throats, maintaining effective permeability. Breakthrough pressure drops to an extremely low value (0.7 MPa), and the sealing capacity of caprock mudstone is severely compromised, exhibiting poor sealing performance (Figure 10).

The medium-to-high temperature stage (600–900 °C): High-temperature softening or partial melting of cementing materials may become more pronounced, accompanied by changes along mineral boundaries and further expansion of transgranular cracks (Figure 4h). The contraction of pore-throat dimensions may be associated with the redistribution and re-solidification of softened cementing phases during cooling, with the dominant pore-throat radii concentrated in the range of 0.063–0.16 µm. Flow capacity significantly weakens, with flow pathways exhibiting a pronounced leftward shift (Figure 5d). High-pressure mercury withdrawal efficiency at 900 °C drops to merely 1.156%, while pore-throat connectivity enhances and permeability surges over threefold. The diffusion coefficient increases abruptly by an order of magnitude, leading to substantial degradation of sealing capacity, ultimately resulting in extremely poor sealing performance (Figure 10).

High-temperature stage (900–1200 °C): Feldspar-bearing and other mineral components may undergo high-temperature structural alteration and local softening, while partial melting of feldspar-rich phases may contribute to the extensive development and interconnection of pores and fractures (Figure 4i) [42–44]. Pore-throat dimensions increase abruptly, with a portion reaching radii of 4–6.3 µm. These pore throats constitute dominant flow pathways, significantly enhancing flow capacity (Figure 5e). At this stage, the sealing capacity of the mudstone caprock is entirely lost, rendering it unsuitable for caprock applications (Figure 10).

4.4. UCG Sealing Mode

During underground coal gasification (UCG), the temperature field of gasification chambers exhibits a defined influence range and spatial distribution characteristics within caprock mudstone. By integrating the sealing characteristics of caprock mudstone with the thermal distribution patterns during UCG, a conceptual model illustrating the distribution characteristics and sealing mechanisms of caprock in the Baikouquan area during UCG processes is developed (Figure 11).

The present measurements were obtained after the specimens had cooled to room temperature and therefore mainly characterize the residual properties of the mudstone after thermal treatment. Under in situ UCG conditions, thermal damage may interact with pore-pressure evolution, stress redistribution, time-dependent deformation, and transient mechanical disturbances. Methodological advances in subsurface geomechanics have shown that poro-elasto-viscoplastic-dynamic formulations can integrate pore-pressure changes, irreversible time-dependent deformation, and dynamic responses within a unified framework [45]. Incorporating these processes into future thermal-hydraulic-mechanical models would provide a more comprehensive assessment of pore-fracture evolution and mudstone caprock integrity during UCG. It also should be noted that only one specimen

was tested for each test item at each temperature. Although all specimens were obtained from the same core column and prepared with the same orientation, the effects of specimen-scale heterogeneity and anisotropy could not be statistically evaluated. Therefore, the observed trends should be interpreted as representative of the core series tested within the study area, and additional replicate tests are required to assess their broader applicability.

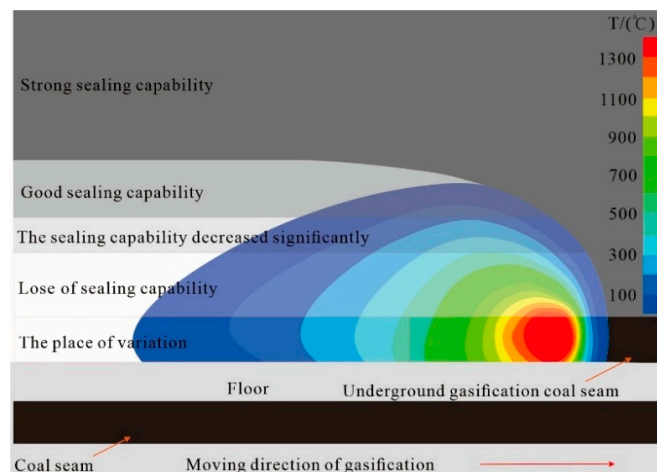


Figure 11. Diagram of the sealing mode of mudstone caprock (Quote from [9]).

5. Suggestions

Given that the temperature during UCG influences the sealing capability of the overlying mudstone, it is suggested that the mudstone affected by temperature and with a temperature below 200 °C be used as an effective caprock for the gasification chamber (Figure 12). This research outcome can offer guidance for the selection of the overlying strata for the UCG chamber in the Baikouquan area and furnish theoretical support for the actual production in this region.

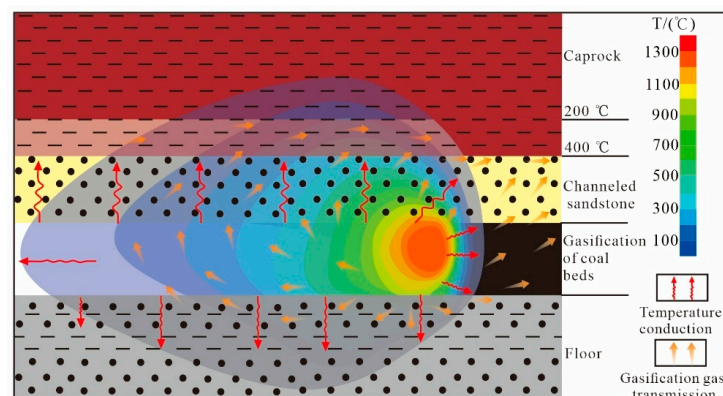


Figure 12. Patterns of heat transfer, gas migration, and caprock sealing during UCG in the Baikouquan area.

6. Conclusions

Thermal exposure progressively reorganizes the pore-fracture network of the mudstone caprock. Integrated SEM, high-pressure mercury intrusion, porosity, permeability, breakthrough pressure, and diffusion coefficient results show that sealing deterioration is controlled by mineral dehydration, thermally induced fracturing, and high-temperature melting. The most pronounced transition occurs near 400 °C, after which the breakthrough pressure remains low and the sealing capacity is severely degraded.

In the low-temperature stage (25–200 °C), the porosity and permeability of the mudstone increases slowly and the pore morphology expands slightly, but the mudstone is not broken, and its sealing capability is not significantly affected by temperature, so the sealing capability is strong. In the low-to-medium temperature stage (200–400 °C), the porosity and permeability of the mudstone increase significantly, and the breakthrough pressure and sealing ability drop sharply. The marked decrease in breakthrough pressure between 300 and 600 °C, together with the microstructural changes observed at 400 °C, supports an approximate critical temperature of 400 °C. During the medium- and high-temperature stages, porosity increases overall, whereas permeability reaches its maximum at 900 °C and then decreases at 1200 °C. Nevertheless, the breakthrough pressure remains low, and the diffusion coefficient exceeds the effective sealing range. These changes indicate severe deterioration of the mudstone caprock sealing capacity.

The variations in the physical properties and sealing capability of the mudstone may be associated with mineral dehydration, thermally induced structural alteration, and high-temperature softening or partial melting processes. Given the impact of temperature on the sealing capability of the caprock during UCG, it is suggested that the mudstone that is affected by temperature at 200 °C or below should be used as an effective caprock for the gasification chamber.

Author Contributions: Conceptualization, X.L., S.S. and Z.H.; Methodology, X.L., S.S. and Z.H.; Software, C.J., X.Y. and W.L.; Validation, C.J., X.Y. and W.L.; Formal analysis, C.J., X.Y., W.L., S.S. and Z.H.; Investigation, C.J., X.Y. and W.L.; Resources, X.L. and S.S.; Data curation, C.J. and X.Y.; Writing—original draft, C.J.; Writing—review and editing, C.J., X.Y. and X.L.; Visualization, C.J., X.Y. and W.L.; Supervision, X.L., S.S. and Z.H.; Project administration, X.L., S.S. and Z.H.; Funding acquisition, X.L. and Z.H. All authors have read and agreed to the published version of the manuscript.

Funding: This study was funded by the Key Research and Development Program of Xinjiang Uygur Autonomous Region (2024B03002), the National Science and Technology Major Project (2024ZD1406000), and the Xinjiang Uygur Autonomous Region “Tianshan Talent” Leading Scientific and Technological Innovation Talent Support Project (2023TSYCLJ0005).

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding authors.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Bhutto, A.W.; Bazmi, A.A.; Zahedi, G. Underground coal gasification: From fundamentals to applications. *Prog. Energy Combust. Sci.* **2013**, *39*, 189–214. [\[CrossRef\]](#)
2. Takyi, S.A.; Zhang, Y.; Si, M.; Zeng, F.; Li, Y.; Tontiwachwuthikul, P. Current status and technology development in implementing low carbon emission energy on underground coal gasification (UCG). *Front. Energy Res.* **2023**, *10*, 1051417. [\[CrossRef\]](#)
3. Korre, A.; Durucan, S.; Nie, Z. Life cycle environmental impact assessment of coupled underground coal gasification and CO₂ capture and storage: Alternative end uses for the UCG product gases. *Int. J. Greenh. Gas Control* **2019**, *91*, 102836. [\[CrossRef\]](#)
4. Wang, G.; Zheng, J.; Liu, Y.; Xin, L. Experimental study on the microstructure change and evolution law of sandstone under different temperatures. *Chin. J. Rock Mech. Eng.* **2024**, *43*, 600–610. (In Chinese) [\[CrossRef\]](#)
5. Akbarzadeh, H.; Chalaturnyk, R.J. Structural changes in coal at elevated temperature pertinent to underground coal gasification: A review. *Int. J. Coal Geol.* **2014**, *131*, 126–146. [\[CrossRef\]](#)
6. Weinbrandt, R.M.; Ramey, H.J., Jr.; Casse, F.J. The effect of temperature on relative and absolute permeability of sandstones. *Soc. Pet. Eng. J.* **1975**, *15*, 376–384. [\[CrossRef\]](#)
7. Zhou, Q.; Zhu, Z.; Zhang, R.; Fan, Z.; Nie, X.; Gao, W.; Li, C.; Wang, J.; Ren, L. Rock fracture initiation under deep extreme in situ conditions: A review. *J. Rock Mech. Geotech. Eng.* **2024**, *16*, 5297–5324. [\[CrossRef\]](#)
8. Li, Y.; Li, J.; Peng, J.; Ge, D.; Bo, K. Effect of artificially induced microcracks near the rock surface on granite fragmentation performance under heating treatment. *Int. J. Rock Mech. Min. Sci.* **2024**, *182*, 105894. [\[CrossRef\]](#)

9. Zhang, Y.; Zhao, G.F.; Li, Q. Acoustic emission uncovers thermal damage evolution of rock. *Int. J. Rock Mech. Min. Sci.* **2020**, *132*, 104388. [\[CrossRef\]](#)
10. Liu, L.; Ji, H.; Elsworth, D.; Zhi, S.; Lv, X.; Wang, T. Dual-damage constitutive model to define thermal damage in rock. *Int. J. Rock Mech. Min. Sci.* **2020**, *126*, 104185. [\[CrossRef\]](#)
11. Xie, Z.; Ling, S.; Liao, X.; Wu, X.; Zhao, S.; Chen, M.; Duan, Q. Study on the weightless-expansion mechanism of red-layer mudstone at different heat treatment temperatures. *Chin. J. Rock Mech. Eng.* **2023**, *42*, 154–167. (In Chinese) [\[CrossRef\]](#)
12. Saif, T.; Lin, Q.; Bijeljic, B.; Blunt, M.J. Microstructural imaging and characterization of oil shale before and after pyrolysis. *Fuel* **2017**, *197*, 562–574. [\[CrossRef\]](#)
13. Saif, T.; Lin, Q.; Butcher, A.R.; Bijeljic, B.; Blunt, M.J. Multi-scale multi-dimensional microstructure imaging of oil shale pyrolysis using X-ray micro-tomography, automated ultra-high-resolution SEM, MAPS Mineralogy and FIB-SEM. *Appl. Energy* **2017**, *202*, 628–647. [\[CrossRef\]](#)
14. Luo, Z.; Duan, Y.; Wang, X.; Zhang, X. Evaluation on sealing performance of mudstone caprocks of gas reservoir-type gas storage in a high-temperature environment. *China Saf. Sci. J.* **2022**, *32*, 74–82. (In Chinese) [\[CrossRef\]](#)
15. Liu, X. Study on high-temperature burnt surrounding rock movement and failure mechanism in underground coal gasification. *Chin. J. Rock Mech. Eng.* **2022**, *41*, 1512. (In Chinese) [\[CrossRef\]](#)
16. Yao, X.; Li, X.; Wei, B.; Tian, J.; Yang, S.; Ju, Y. Numerical simulations of fracture propagation in overlying strata for deep underground coal gasification using controlled retraction injection point technology. *Energy* **2025**, *317*, 134684. [\[CrossRef\]](#)
17. Ekneligoda, T.C.; Marshall, A.M. A coupled thermal-mechanical numerical model of underground coal gasification (UCG) including spontaneous coal combustion and its effects. *Int. J. Coal Geol.* **2018**, *199*, 31–38. [\[CrossRef\]](#)
18. Wang, J.; Wang, Z.; Xin, L.; Xu, Z.; Gui, J.; Lu, X. Temperature field distribution and parametric study in underground coal gasification stope. *Int. J. Therm. Sci.* **2017**, *111*, 66–77. [\[CrossRef\]](#)
19. Fang, H.; Liu, Y.; Ge, T.; Zheng, T.; Yu, Y.; Liu, D.; Ding, J.; Li, L. A review of research on cavity growth in the context of underground coal gasification. *Energies* **2022**, *15*, 9252. [\[CrossRef\]](#)
20. Yang, D.; Sarhosis, V.; Sheng, Y. Thermal-mechanical modelling around the cavities of underground coal gasification. *J. Energy Inst.* **2014**, *87*, 321–329. [\[CrossRef\]](#)
21. Otto, C.; Kempka, T. Thermo-mechanical simulations of rock behavior in underground coal gasification show negligible impact of temperature-dependent parameters on permeability changes. *Energies* **2015**, *8*, 5800–5827. [\[CrossRef\]](#)
22. Lozynskyi, V. Numerical simulation of carbonaceous raw material combustion in a coal seam channel. *Min. Miner. Depos.* **2024**, *18*, 109–124. [\[CrossRef\]](#)
23. Gao, W.; Zagorščak, R.; Thomas, H.R. Insights into solid-gas conversion and cavity growth during underground coal gasification (UCG) through thermo-hydraulic-chemical (THC) modelling. *Int. J. Coal Geol.* **2021**, *237*, 103711. [\[CrossRef\]](#)
24. Saik, P.; Lozynskyi, V.; Berdnyk, M.; Klimov, D. Dynamics of temperature-strength changes in the immediate roof and formation of the gasified cavity of an underground gasifier. *Eng. J. Satbayev Univ.* **2026**, *148*, 16–28. [\[CrossRef\]](#)
25. Zhu, Z.; Li, Q.; Chen, H.; Li, J.; Zhang, W.; Liu, Y.; Yan, Z. Tectonic-geomorphological evolution and provenance-sedimentary response: Insights from the Middle Jurassic–Lower Cretaceous, Junggar Basin, China. *Mar. Pet. Geol.* **2023**, *158*, 106514. [\[CrossRef\]](#)
26. Huang, L.; Su, J.; Pan, S.; Li, C.; Wang, Z. Tectonic evolution of the early Permian Junggar Basin: Insights into a foreland basin shaped by lithospheric folding. *Mar. Pet. Geol.* **2025**, *171*, 107178. [\[CrossRef\]](#)
27. Zhang, W.; Sun, Q.; Hao, S.; Geng, J.; Lv, C. Experimental study on the variation of physical and mechanical properties of rock after high-temperature treatment. *Appl. Therm. Eng.* **2016**, *98*, 1297–1304. [\[CrossRef\]](#)
28. Pathiranagei, S.V.; Gratchev, I.; Kong, R. Engineering properties of four different rocks after heat treatment. *Geomech. Geophys. Geo-Energy Geo-Resour.* **2021**, *7*, 16. [\[CrossRef\]](#)
29. Washburn, E.W. The dynamics of capillary flow. *Phys. Rev.* **1921**, *17*, 273–283. [\[CrossRef\]](#)
30. SY/T 5748-2020; Determination Method of Gas Breakthrough Pressure in Rock. Petroleum Industry Press: Beijing, China. 2020.
31. Chen, B.; Li, Q.; Tan, Y.; Yu, T.; Li, X.; Li, X. Experimental measurements and characterization models of caprock breakthrough pressure for CO₂ geological storage. *Earth-Sci. Rev.* **2024**, *252*, 104732. [\[CrossRef\]](#)
32. Zhang, J.; Liu, G.; Torsaeter, O.; Tao, S.; Jiang, M.; Li, G.; Zhang, S. Pore-throat structure characteristics and their effect on flow behavior in the Gaotaizi tight siltstone reservoir, northern Songliao Basin. *Mar. Pet. Geol.* **2020**, *122*, 104651. [\[CrossRef\]](#)
33. Al-Bazali, T.M.; Zhang, J.; Chenevert, M.E.; Sharma, M.M. Measurement of the sealing capacity of shale caprocks. In Proceedings of the SPE Annual Technical Conference and Exhibition, Dallas, TX, USA, 9–12 October 2005; SPE-96100-MS. [\[CrossRef\]](#)
34. Mouzakis, K.M.; Navarre-Sitchler, A.K.; Rother, G.; Bañuelos, J.L.; Wang, X.; Kaszuba, J.P.; Heath, J.E.; Miller, Q.R.S.; Alvarado, V.; McCray, J.E. Experimental study of porosity changes in shale caprocks exposed to CO₂-saturated brines I: Evolution of mineralogy, pore connectivity, pore size distribution, and surface area. *Environ. Eng. Sci.* **2016**, *33*, 725–735. [\[CrossRef\]](#)
35. Yuan, M.; Jing, Y.; Lanetc, Z.; Zhuravljov, A.; Soleimani, F.; Si, G.; Armstrong, R.T.; Mostaghimi, P. Modelling multicomponent gas diffusion and predicting the concentration-dependent effective diffusion coefficient of coal with application to carbon geo-sequestration. *Fuel* **2023**, *339*, 127255. [\[CrossRef\]](#)

36. Liu, Z.; Emami-Meybodi, H. Apparent diffusion coefficient for adsorption-controlled gas transport in nanoporous media. *Chem. Eng. J.* **2022**, *450*, 138105. [[CrossRef](#)]
37. Espinoza, D.N.; Santamarina, J.C. CO₂ breakthrough—Caprock sealing efficiency and integrity for carbon geological storage. *Int. J. Greenh. Gas Control* **2017**, *66*, 218–229. [[CrossRef](#)]
38. Pang, Y.; Soliman, M.Y.; Deng, H.; Xie, X. Experimental and analytical investigation of adsorption effects on shale gas transport in organic nanopores. *Fuel* **2017**, *199*, 272–288. [[CrossRef](#)]
39. Hildenbrand, A.; Schlömer, S.; Krooss, B.M. Gas breakthrough experiments on fine-grained sedimentary rocks. *Geofluids* **2002**, *2*, 3–23. [[CrossRef](#)]
40. Valášková, M.; Blahůšková, V.; Vlček, J. Effects of kaolin additives in fly ash on sintering and properties of mullite ceramics. *Minerals* **2021**, *11*, 887. [[CrossRef](#)]
41. Ge, W.; Mao, H.; Chen, J.; Min, F.; Liu, H.; Song, S. Understanding the thermal activation behavior of montmorillonite and kaolinite at the atomic level by ReaxFF molecular dynamics simulations. *Appl. Clay Sci.* **2024**, *251*, 107313. [[CrossRef](#)]
42. Viani, A.; Cultrone, G.; Sotiriadis, K.; Ševčík, R.; Šásek, P. The use of mineralogical indicators for the assessment of firing temperature in fired-clay bodies. *Appl. Clay Sci.* **2018**, *163*, 108–118. [[CrossRef](#)]
43. Romero, M.; Padilla, I.; Contreras, M.; Lopez-Delgado, A. Mullite-based ceramics from mining waste: A review. *Minerals* **2021**, *11*, 332. [[CrossRef](#)]
44. Wang, S.; Gainey, L.; Wang, X.; Mackinnon, I.D.; Xi, Y. Influence of palygorskite on in situ thermal behaviours of clay mixtures and properties of fired bricks. *Appl. Clay Sci.* **2022**, *216*, 106384. [[CrossRef](#)]
45. Guo, X.; Jin, Y.; Miu, T.; Wei, S.; Xia, Y.; Tang, J. Investigation of the time-dependent and dynamic geomechanical behaviors induced by depressurization in natural gas hydrate-bearing sediments based on a poro-elasto-viscoplastic-dynamic model. *Int. J. Rock. Mech. Min. Sci.* **2026**, *197*, 106357. [[CrossRef](#)]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.