The Fracture and Energy of Coal Evolution under Thermo-Mechanical Coupling via a Particle Flow Simulation

Yongsheng Gu 1, Lei Song 1,*, Lei Zhang 2, Xiangyu Wang 3 and Zhenbo Zhao 1

1 School of Energy and Mining Engineering, China University of Mining and Technology, Beijing 100083, China
2 College of Safety and Emergency Management Engineering, Taiyuan University of Technology, Taiyuan 030024, China
3 School of Mechanics and Civil Engineering, China University of Mining and Technology, Beijing 100083, China
* Correspondence: songlei_leo@126.com

Abstract: The increase in mining depth causes the temperature of the coal seam to rise. Studying the effect of temperature on the mechanical property of coal is very necessary. In this paper, based on the results of conventional triaxial compression experiments of coal samples, the discrete element program PFC2D was used to conduct a conventional triaxial compression simulation of coal samples to obtain microscopic parameters. On this basis, the conventional triaxial simulation study of coal samples at different temperatures was carried out to explore the influence of temperature on the physical and mechanical properties of coal. In this process, acoustic emission and energy monitoring were carried out. The damage and failure process of coal is divided into three stages: the undamaged stage, the stable damage stage, and the rapid damage stage. The relationship between acoustic emission characteristic law, energy transformation law, and crack evolution in the damage and failure process of coal was analyzed in detail. The results indicate that the fracture evolution is affected by the increase in cross-sectional area and the decrease in distance between particles due to the expansion of particles, which corresponds to the phenomenon that the temperature increase produces new microcracks and the particles expand to fill the original cracks in the experiment. This indicates that PFC2D can be used as an effective numerical method for a coal mesoscopic study, and the results of these numerical experiments are also helpful to deepen the understanding of the damage mechanism of coal failure under thermo-mechanical coupling.

Keywords: particle flow simulation; temperature; three-axis; acoustic emission; energy

1. Introduction

The mining conditions of coal in China are extremely complex and are seriously threatened by high-temperature heat damage, and 53% of the detected coal resources are buried below 1000 m [1]. The increase in mining depth leads to the rise of ground temperature. Therefore, many scholars have completed a lot of research on the change in physical and mechanical properties of coal caused by temperature change. Wang et al. [2] found that thermal stress generated by temperature shock exceeded the tensile strength of coal samples, which was the direct cause of fracture initiation, expansion, and mutual penetration. Through CT scanning, it has been shown that temperature has an obvious influence on the surface and internal fracture structure of coal. Xu et al. [3] carried out triaxial compression experiments of gas-containing coal under different temperature conditions and found that the triaxial compressive strength, residual strength, and elastic modulus showed a gradual decrease trend, but the decrease was slow when the temperature was between 20 °C and 60 °C, and the decrease was rapid when the temperature was over 60 °C. Zhang et al. [4] studied the influence of a normal temperature of 800 °C on the mechanical properties of marble and showed that the increase in temperature reduced the peak strength and elastic modulus of marble to different degrees.
When the coal material is subjected to the external load, its internal stress concentration will occur. When the stress reaches the critical value, cracks will occur in the coal. During this process, energy will be generated to release and spread around in elastic and stress waves. The acoustic emission phenomenon is the precursor information of coal compression fracture instability, so it is widely used in mining, tunnel, slope, and another geotechnical engineering. According to the Kaiser effect, AE activity increases sharply when rocks exceed the previous maximum stress level [5]. Goodman [6] found through the acoustic monitoring of coal, sandstone, and diorite in the loading process that acoustic interference was always accompanied by a specific stress level, which proved the Kaiser effect to a certain extent. Pestman et al. [7] conducted a series of laboratory acoustic emission experiments on sandstone under a triaxial compression load. The results showed that the state of surface rocks had an impact on the acoustic emission signal law. Xie et al. [8] pointed out that energy plays a fundamental role in the process of rock failure through uniaxial compression experiments on different kinds of rocks, which can well describe the deformation and failure of rocks from the perspective of energy. Pei et al. [9] carried out a study on AE characteristics and energy evolution of granite under uniaxial compression. The results showed that the combination of AE characteristics and energy evolution could effectively improve the prediction accuracy of rock failure. M. Cai et al. [10] adopted the finite difference method (FLAC) and discrete element (PFC) coupling modeling, PFC modeling was used to model the rock mass around the AE sensor, and FLAC modeling was used to model the rest of the rock mass. This method was used to simulate the AE activity at the position of the AE sensor in Kannagawa chamber. The results were in good agreement with the on-site monitoring results.

As a two-dimensional discrete element software, PFC2D discretizes the object into a certain number of particle units and gives them unique properties based on Newton’s second law. The main contact modes of particles in the program are linear contact bonding and linear parallel bonding. The linear parallel bond model can transmit shear force, normal force, and bending moment simultaneously. This method is widely used to simulate the mechanical properties of rock-like materials [11,12]. Su et al. [13] used PFC2D to study the spatio-temporal characteristics of acoustic emissions from a mesoscopic perspective. As a result, the strain energy is absorbed during the calm period of AE by strain energy tracing, and there is healing in the failure process of surface rock. Zhou et al. [14] compared the acoustic emission characteristics of the whole process of granite fracture in the chamber with the computational simulation results and verified the reliability of this method. It is also shown that the number of AE events is approximately normally distributed with the change in fracture strength.

It can be seen that previous researchers have completed a lot of work on laboratory experiments of thermo-mechanical coupling and acoustic emission-related numerical experiments.

However, there are few numerical simulation experiments on the acoustic emission of coal and the energy conversion in the process under the thermo-mechanical coupling condition. Based on previous studies, this paper carried out particle flow simulation experiments under thermal-mechanical coupling conditions. The acoustic emission characteristics, energy evolution trend, and fracture evolution law were observed simultaneously. The cracks were divided into shear cracks and tensile cracks. The whole process of crack evolution and the effect of temperature on crack evolution were studied. The paper provides a numerical method to further study the physical and mechanical properties of coal in simulation experiments under thermo-mechanical coupling conditions.

2. Model Construction and Parameter Calibration

2.1. Model Construction

Coal samples were collected from the 28802-working face of No. 8 coal at Dongqu CoalMine in Taiyuan City, Shanxi Province. The coal seam is 400 m beneath the surface. The density of coal is about 1400 kg/m³. To study the mechanical properties of coal samples,
four groups of 25 mm diameter and 50 mm height samples were prepared for conventional triaxial compression experiments. In addition, the in situ stress is about 10 MPa at a depth of 400 m. The actual confining pressure in the mining process is less than 10 MPa. So, we set a confining pressure gradient of 3, 5, 6, and 7 MPa. The loading rate was set to 0.1 m/s. The specific sample size and other physical parameters and test program are shown in Table 1.

Table 1. Physical parameters and experimental schemes of the coal samples.

<table>
<thead>
<tr>
<th>Rock Sample Number</th>
<th>Diameter/mm</th>
<th>Height/mm</th>
<th>Density/(kg m⁻³)</th>
<th>Confining Pressure/MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>D-01</td>
<td>24.9</td>
<td>50.1</td>
<td>1400.6</td>
<td>3</td>
</tr>
<tr>
<td>D-02</td>
<td>24.9</td>
<td>50.1</td>
<td>1400.3</td>
<td>5</td>
</tr>
<tr>
<td>D-03</td>
<td>24.8</td>
<td>50.2</td>
<td>1399.8</td>
<td>6</td>
</tr>
<tr>
<td>D-04</td>
<td>24.9</td>
<td>49.9</td>
<td>1399.6</td>
<td>7</td>
</tr>
</tbody>
</table>

In this paper, the connection mode between particles was set as parallel bonding (Figure 1). The linear part of the parallel bond model does not resist relative rotation and accommodates sliding by applying the Coulomb limit of shear force [15]. In the test, a servo mechanism was used to control the left and right walls to keep the confining pressure unchanged. The loading was carried out in the way of controlled displacement.

In the above figure, $k_a$, $k_s$ are linear stiffness, $\bar{k}_a$, $\bar{k}_n$ are the stiffness of the parallel bonding part, $\mu$ is the friction coefficient, $\bar{c}$ is the cohesion, and $\phi$ is the angle of internal friction.

2.2. Mesoscopic Parameter Calibration

The equipment used in this triaxial experiment was the GCTS rock experiment system, which is a multi-functional rigid pressure device specially designed for rock experiments under electro-hydraulic servo control. It is equipped with automatic pressure and measurement system under servo control. The numerical simulation experiments were completely consistent with the laboratory experimental conditions. The conventional triaxial tests with confining pressures of 3, 5, 6, and 7 MPa were carried out, respectively. The basic method of the trial-and-error method by writing a python program faster satisfied the basic demands of macro parameters to make the microscopic parameters. The simulation experiment and laboratory experiment of the partial stress–strain curve (Figure 2), peak strength as the confining pressure change trend (Figure 3), and crack figure were compared (Figure 4). The mesoscopic parameters are shown in Table 2. The results show that the numerical simulation results of PFC²D were very close to the laboratory experimental results.
Processes 2022, 10, x FOR PEER REVIEW 4 of 16

completely consistent with the laboratory experimental conditions. The conventional triaxial tests with confining pressures of 3, 5, 6, and 7 MPa were carried out, respectively. The basic method of the trial-and-error method by writing a python program faster satisfied the basic demands of macro parameters to make the microscopic parameters. The simulation experiment and laboratory experiment of the partial stress–strain curve (Figure 2), peak strength as the confining pressure change trend (Figure 3), and crack figure (Figure 4) were compared (Figure 4). The mesoscopic parameters are shown in Table 2. The results show that the numerical simulation results of PFC2D were very close to the laboratory experimental results.

Table 2. Micro-parameters in PFC2D.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values</th>
<th>Parameter</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum radius/mm</td>
<td>0.3</td>
<td>Cohesion (stress)/MPa</td>
<td>11.86</td>
</tr>
<tr>
<td>Maximum radius/mm</td>
<td>0.45</td>
<td>Tensile strength (stress)/MPa</td>
<td>23.72</td>
</tr>
<tr>
<td>Effective modulus(force/area)/GPa</td>
<td>1.42</td>
<td>Friction angle (degrees)</td>
<td>65.41</td>
</tr>
<tr>
<td>Normal-to-shear stiffness ratio</td>
<td>1.5</td>
<td>Friction coefficient</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Figure 2. Numerical and experimental results under different confining pressures.

Figure 3. Numerical and experimental peak stresses at different confining pressures.
3. Triaxial Simulation Experiment under Thermal-Mechanical Coupling Conditions

3.1. Mathematical Model Description

The heat conduction material in PFC\textsuperscript{2D} is composed of a heat storage medium and a heat transfer pipe (Figure 5). The particles are the heat storage medium, and the contact between the particles is the heat transfer pipe. The displacement and stress changes caused by temperature were simulated by assigning a particle thermal expansion coefficient and particle interaction in temperature change [16]. The thermal expansion radius can be calculated from the following equation:

$$\Delta R = a R \Delta T$$

(1)

where $a$ is the particle thermal expansion coefficient, $R$ is the particle radius, and $\Delta T$ is the temperature increment.

![Figure 4. Numerical and experimental cracks under different confining pressures.](image)

![Figure 5. Heat conduction diagram.](image)
PFC$^{2D}$ stipulates that the normal component of the force vector carried in the parallel contact model is used as the heat transfer channel. At the same time, assuming isotropic expansion of the material to effectively change the bonding length, the calculation formula of this model is:

$$\Delta F_n = -k_n A \Delta U_n = -k_n A (\pi l \Delta T)$$  \hspace{1cm} (2)

where: $\Delta F_n$ is the normal component of the force at the bonding; $k_n$ is the normal stiffness; $\pi$ is the thermal expansion coefficient of the bond material; $l$ is the bond length; $T$ is the temperature variation; $A$ is the cross-sectional area at the bonding; $\Delta U_n$ is the normal displacement increment of this equation of the “Contact Resolution” section.

According to the empirical value, $9 \times 10^{-6}$ k$^{-1}$ was used as the thermal expansion coefficient in the numerical model [17]. The four walls were heated uniformly, and the heating degree was controlled by heat transfer time until the whole numerical model reached the preset temperature. The heating process is shown in Figure 6. The ground temperature increased with the increase in mining depth. According to the monitoring data of the working face, 30, 50, and 70 °C could be achieved. The predicted temperature was 90 °C. The four temperature gradients including 30, 50, 70, and 90 °C were set to carry out a conventional triaxial simulation experiment with confining pressure of 5 MPa. Acoustic emission monitoring and energy tracking were carried out during this process.

![Figure 6. Coal sample heating process.](image)

### 3.2. Numerical Simulation Results

In the laboratory experiment, acoustic emission technology was coupled to the test piece by the sensor, through which the signal was received and amplified. The number of pulses per unit of time was the counting rate, and the total number of pulses was the total number of AE [18,19].

The basic principle of AE in PFC$^{2D}$ is to specify a unit time or unit strain in the process of sample compression. Through its program, the newly generated microcracks are counted in unit time or unit strain to obtain the situation of the generation of microcracks in a certain period [20]. Through the triaxial compression simulation experiment of coal samples under four temperature gradients of 30, 50, 70, and 90 °C, the results as shown in the figure below were obtained.

### 3.3. Law of Acoustic Emission

To better analyze the law of damage and failure process of coal samples, this process was divided into three stages: undamaged stage, damage stable development stage, and damage rapid development stage [21,22]. In the undamaged stage, due to the existence of primary pore cracks, these pore cracks were compacted and closed under the joint action of axial pressure and confining pressure, and almost no acoustic emission signals were
generated at this stage. With the further compression of the pore and crack structure, the sample reached a compact state, and the energy was accumulated. At this time, micro-cracks began to occur locally, and a small number of acoustic emission signals were released. In this process, the AE events were relatively stable, and occasionally the AE events increased. In the rapid damage stage, AE became more active. In this stage, new cracks were formed in the coal samples, which continued to develop and extended into macroscopic cracks. The coal was seriously damaged, and the AE phenomenon was very active.

This indicates that the development of microcracks promoted the failure of rocks, and after the failure of rocks, more microcracks were generated. After the instability and rupture of coal samples, the axial deformation increased sharply and the axial stress decreased rapidly. Due to friction and slip on the fracture surface or between particles, there was still a small amount of acoustic emission activity.

According to the deformation and failure process of coal samples, the cumulative AE curve was also divided into three stages: the stable AE stage, the stable AE rising stage, and the rapid AE rising stage [23]. Figure 7 shows that the AE cumulative number in the calm phase was horizontal and straight, and the cumulative number was almost 0. In this process, the primary pores were closed under external load, AE events and cumulative AE events were very few, and the AE signals were very weak.

![Deviator stress-strain curve](image1)

![Number of AE events](image2)

![Accumulated AE count](image3)

**Figure 7.** Deviatoric stress, number of AE events, and accumulated AE count versus axial strain.

**30 °C**

**50 °C**

**70 °C**

**90 °C**
However, as the temperature rose, AE signals appeared earlier. In the stable rising stage, the number of AE events at each temperature increased compared with the previous stage, and the slope was almost unchanged. With the increase in temperature, the number of AE events and the cumulative number of AE events both showed an increasing trend. We noticed that the cumulative AE number reached 1978 when the temperature was 50 °C, which was higher than 1668 at 30 °C, 1739 at 70 °C, and 1834 at 90 °C. It can be explained that when the temperature increases, the particle radius expands, which increases the cross-section of the cementation but also decreases the cementation length. Although the strength was slightly larger than that at 70 °C, it is more likely to produce relative displacement and cause cementation failure due to the greater relative contact between particles. In other words, under the condition that the strength decreased with the increase in temperature, the number of cracks produced at 50 °C was more affected by the increase in cross-section, which was also confirmed by the monitoring of the number of tensile cracks (Figure 8). Laboratory experiments also can appear in similar situations [24] which can be interpreted when the temperature is a higher relative increment.

![Figure 8. Variation of peak stress with temperature and crack distribution under peak stress at 5 MPa.](image_url)

The expansion of the particle made the coal sample develop new cracks due to the temperature and the particles filled the hole fissure between the original, although the overall strength of the specimens declined slightly. However, the concept of the micro-crack number instead appeared relatively decreased. To verify the above, we continued to carry out gradient experiments with confining pressures of 3, 6, 7 MPa, and the results showed the same trend (Figure 9).

Comparing the compressive strength of coal samples at different temperatures, it is easy to find that the compressive strength of coal samples decreased with the increase in temperature, and the change was small between 30 and 70 °C. The peak intensity decreased significantly at 90 °C, which decreased by 1.31 MPa compared with that at 70 °C.
to carry out gradient experiments with confining pressures of 3, 6, 7 MPa, and the results showed the same trend (Figure 9).

Figure 8. Variation of peak stress with temperature and crack distribution under peak stress at 5 MPa.

Figure 9. Variation of peak stress with temperature under different confining pressures.

3.4. Law of Energy Evolution

Rocks are subjected to external loads, accompanied by energy input, conversion, release, and dissipation. Many scholars have analyzed the damage process of rock according to the energy transformation. The relationship between rock damage and failure process and energy transformation has been extensively studied [25–27]. However, most of the current studies focused on energy transformation at a specific stage, and the transformation of input energy, elastic energy, and dissipated energy in the whole process was less [28].

In particular, there is a lack of corresponding technical means to visualize the evolution of microcracks in the process of energy evolution. In addition, the calculation of elastic energy and dissipative energy in real experiments has been obtained by the stress–strain curve calculation [29]. For the regulation of the unloading point, the human influence factor is large. Due to its unique advantages in real-time performance and visualization, numerical methods can be used to support each other with real experiments to better study the specific relationship between energy evolution and rock damage and failure process.

Four energy forms are specified in the parallel bond model of PFC2D. They are the strain energy stored in the linear spring, the friction energy dissipated by friction and slip, the damping energy dissipated by the damper, and the bonding strain energy stored in the parallel cemented spring seat, respectively [30]. Because the loading method in this paper was quasi-static loading, the kinetic energy of the particles was neglected. To understand the energy evolution, in this paper, the strain energy in linear spring and the strain energy in parallel cemented spring were synthesized as strain energy. The dissipated damping energy in the damper and the frictional energy generated by particle friction slip were unified as dissipated energy.

Figure 10 shows that the change trends of input energy, elastic strain energy, and dissipated energy of coal samples during loading were the same under different temperature conditions. In the undamaged stage of the coal sample, the input energy and elastic energy curve coincided. The dissipated energy was almost zero and remained unchanged. When coal entered the damage stable development stage, the input energy and elastic energy curves grew faster, and the dissipated energy continued to develop slowly, indicating that the energy transformation in this stage was still dominated by elastic energy. In the rapid development stage after injury, because of the new hole crack production and expansion, the slope of the dissipated energy curve increased, but the peak value of each energy curve...
lagged behind the peak stress. This is because the larger macro fracture was not formed, and the elastic energy could not start a large number of releases.

![Deviator stress-strain and energy evolution curves](image1)

**Figure 10.** Deviatoric stress–strain and energy evolution curves.

This was mutually verified with the AE event peak lagging behind the peak intensity. The micro-cracks extended into macroscopic cracks and failure surfaces, and the sample was divided into coal blocks (Figure 11). The elastic energy stored in the coal body was released in large quantities, which was converted into the friction energy between coal blocks and the friction energy in the damper, namely the dissipative energy specified in this paper.

![Destruction of the fragment](image2)

**Figure 11.** Destruction of the fragment.
With the increase in temperature, the overall input energy decreased, the axial strain corresponding to the increase in dissipative energy advanced, and the peak elastic potential energy decreased. However, the peak strength of elastic potential energy at 50 °C was the same as that at 30 °C, and only the input energy and dissipated energy increased. Thus, the overall trend of energy evolution was consistent with the acoustic emission characteristics.

3.5. Microscopic Fracture Evolution Law

The following rules were obtained after the statistics of the microscopic crack types: at the early stage of AE, the number of tensile cracks and shear is very small. In the stable development stage of AE, almost only shear cracks occurred (Figure 12), but the closer to the peak intensity, the faster the tensile crack occurred. The distribution of tensile cracks was mainly on the macroscopic fracture plane, and with the increase in temperature, both tensile cracks and shear cracks tended to increase, but the increase in tensile cracks was greater than that of shear cracks, and the proportion of tensile cracks in the total cracks also increased (Table 3).

Table 3. Crack distribution at different temperatures.

<table>
<thead>
<tr>
<th>Temperature</th>
<th>30 °C</th>
<th>50 °C</th>
<th>70 °C</th>
<th>90 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crack types</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>shear</td>
<td>1273</td>
<td>1477</td>
<td>1326</td>
<td>1397</td>
</tr>
<tr>
<td>tensile</td>
<td>395</td>
<td>501</td>
<td>413</td>
<td>437</td>
</tr>
<tr>
<td>Total crack number</td>
<td>1668</td>
<td>1978</td>
<td>1739</td>
<td>1834</td>
</tr>
<tr>
<td>Tensile/shear</td>
<td>0.310</td>
<td>0.339</td>
<td>0.311</td>
<td>0.313</td>
</tr>
</tbody>
</table>

Figure 13 shows the damage after the contact distribution state, according to the direction of the tangent vector drawing the contact composition distribution group (Figure 14). It can be seen that the contact distribution was relatively uniform before loading. The contact decreased more along the macroscopic shear plane direction after failure; this method could be used to further study the anisotropic damage of coal caused by an external load. With the increase in temperature (Figure 15), the amount of contact reduction gradually increased, which was consistent with the characteristics of AE and the law of energy evolution.
Figure 13. Contact distribution after failure.

Figure 14. Contact distribution configuration.
Figure 15. Contact configuration distribution after loading at different temperatures.

4. Conclusions

Based on the triaxial compression results of coal samples, using particle flow procedures for 30, 50, 70, and 90 °C, four triaxial compression simulations of the temperature gradient were completed. The process was carried out by acoustic emission monitoring, and energy analysis of the coal under different temperature evolution characteristics of acoustic emission and energy as well as the development of micro cracks and a series of microscopic behavior. The following conclusions were obtained from the numerical simulation results:

(1) The particle flow code had a good effect on the study of microcrack evolution and various mechanical behaviors in the process of coal rock damage and failure. The simulation results included deviatoric stress–strain curves, and the peak strength and microcrack crack development under different confining pressures were consistent with the laboratory experimental results;

(2) The cumulative AE curve was divided into three stages: the stationary stage, the stable ascending stage, and the rapid ascending stage. The dissipated energy curve was horizontal and almost zero in the stationary stage, and the slow growth of dissipated energy corresponded to the steady rise stage. In the rapid growth stage of the AE cumulative curve, the dissipated energy also showed explosive growth. With the increase in temperature, the peak stress of the coal samples decreased, the AE signals were generated in advance, the cumulative AE number increased, and the input energy required for the overall failure of coal and rock decreased;

(3) In the stable ascending stage, shear cracks were the main microcracks, and until the rapid ascending stage, tensile cracks were faster and mainly appeared on the macroscopic shear plane. The increase in temperature led to an increase in tensile cracks, and the proportion of the total number of cracks also increased;

(4) In the process of temperature rise, there was a joint effect of particle expansion, which increased the cross-sectional area between particles and decreased the distance between particles. This led to a certain temperature interval in the experiment, which caused the tensile crack to increase significantly so that the input energy required for failure increased. In the laboratory experiment, these results could be explained by the joint effect of new microcracks generated and the particle expansion to fill the original cracks caused by the temperature rise.
Author Contributions: Y.G.: Writing−original draft; L.S. and Y.G.: numerical simulations; X.W.: review and methodology; L.Z.: analyzed the data; Z.Z.: Software. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the National Natural Science Foundation of China (51827901, 52121003, 52142302), the 111 Project (B14006), the Yueqi Outstanding Scholar Program of CUMTB (2017A03), and the Fundamental Research Funds for the Central Universities (2022YJSNY13).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

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

References


