PFC Numerical Simulation Study of Thermal-mechanical Coupling of Sandstone under Unidirectional Heating

Lin Xin¹, ², *, Mingyu An¹, Mingze Feng¹, Weimin Cheng¹, ², Kaixuan Li¹, Jing Wu¹, Jiaze Li¹

¹College of Safety and Environmental Engineering, Shandong University of Science and Technology, Qingdao, Shandong 266590, China
²Key Laboratory of Ministry of Education for Mine Disaster Prevention and Control, Shandong University of Science and Technology, Qingdao, Shandong 266590, China
Corresponding author: xinlin@sdust.edu.cn

Abstract. In order to study the rock thermal cracking law of the roof rock in the combustion zone of underground coal gasification under the special condition of unidirectional heating, the PFC particle flow software was used to carry out the numerical simulation of thermal-mechanical coupling. The uniaxial compression experiment was used to complete the PFC parameter calibration, establish a mechanical model, and compare the results of the unidirectional heating test with the simulation results. It was found that the relationship between the temperature at the measuring point, the thermal stress and the heating time of the two is very similar. It shows that the simulation results are highly accurate. The simulation results are as follows: when the model is at 450℃ and 600℃, larger-scale cracks are formed and the second larger-scale crack evolution occurs; acoustic emission simulation can be divided into three stages: the first peak stage, the energy accumulation stage, and the second stage. In the second peak stage, the number of model cracks increases with the increase in temperature, and the shear cracks are the main ones, indicating that the model will expand laterally after being subjected to thermal stress, mainly occurring shear failure.

1. Introduction

Underground Coal Gasification (UCG) is a method of controlled combustion of in-situ coal seams and using thermochemical methods to convert them into the required gas[1-3]. In the combustion zone during UCG, the roof rock is in a special state of unidirectional heating, and the roof rock has a small thermal conductivity, short heating time, and a large temperature gradient. The surface moves and the boundary temperature changes dynamically, so the thermal damage of the roof rock also has a gradient change law. If the thermal damage of the rock is too large, coupled with the unreasonable design of the width of the combustion zone, the rock will collapse in a large area and affect the operation of underground coal gasification.

Many scholars have studied the thermal cracking laws of rocks through experiments and numerical simulations. Xu[4] used PFC3D to complete the uniaxial and triaxial test research under high temperature. Wu et al.[5] used finite element and discrete element software to simulate the transient heat conduction in fractured rock. Huang et al.[6] used granite samples with pre-existing defects to be heated to different high temperatures and subjected to uniaxial compression to study the strength evolution and cracking process of thermally damaged rocks. Ali et al.[7] used simulation to analyze the changes in thermal damage. The results show that the particle size greatly affects the simulation results,
and the simulation must be performed under the same particle size. Zhai et al.\cite{8} established a thermo-solid coupling model and used FLAC to perform numerical simulations. They found that high-temperature rock ruptures are due to the heterogeneity of rock components, which leads to heterogeneity in temperature, stress and deformation fields. Li\cite{9} used PFC software to study the changes of granite at different temperatures under ultrasonic vibration.

However, many scholars used the overall heating test method, ignoring that the roof rock in the combustion zone was unidirectionally heated during the UCG. Therefore, this paper used PFC to complete the numerical simulation of thermal-mechanical coupling, and then summarized the thermal cracking law of sandstone under unidirectional heating.

2. Numerical test and parameter calibration

2.1. Uniaxial compression experiment

Since we choose the particle flow software PFC for numerical simulation, we need to establish a model with similar mechanical properties to sandstone samples through parameter calibration, so we obtained the mechanical parameters of sandstone through uniaxial compression experiments. A standard sandstone sample with a size of $\Phi 50\text{mm} \times 100\text{mm}$ was selected, and the uniaxial compression experiment was carried out at a loading speed of 0.01mm/s, and the stress-strain curve diagram is shown in Fig.1.

![Stress-strain curve](image)

Combined with the stress-strain curve diagram, the macroscopic physical and mechanical parameters such as elastic modulus and compressive strength were obtained, as shown in Table 1.

| Table 1 Rock mechanics parameters |
|-----------------------------------|
| Compressive strength /MPa | Elastic Modulus /GPa | Poisson's ratio |
| 54.60 | 5.92 | 0.238 |

2.2. Unidirectional heating test

A self-made unidirectional heating test device in the laboratory was used to complete the heating test of sandstone samples at 150°C-600°C. The test device is shown in Fig.2.
The relationship between temperature, thermal stress and heating time at different heights can be obtained using thermocouples and pressure gauges. As shown in Fig.3 below, only the relationship from 450°C to 600°C was listed.

2.3. Parameter calibration
In order to ensure the high accuracy of the PFC numerical simulation results, it is necessary to calibrate the parameters to make the model and the sample have the same mechanical properties. By continuously adjusting the meso-parameters for numerical simulation, the model parameters that were close to the mechanical properties of the real sample were obtained, as shown in Table 2.

Fig.4 shows that the stress-strain curves obtained from the experiment and simulation were close. The reason why the elastic modulus of the experiment first decreased and then increased was that there were cracks inside the sandstone sample. The initial load was applied to make the particles compact and the cracks compressed.
Table 2 Mesoscopic parameters

| $E^*/$GPa | $E^*/$GPa | $k^*$ | $k^*$ | $p_{b\_ten}$/MPa | $p_{b\_coh}$/MPa | $\mu$ |
|---------|---------|------|------|------------------|-----------------|------|
| 2.15    | 2.25    | 1.7  | 2.15 | 22.2             | 22.2            | 0.5  |

Fig. 4 Comparison diagram of uniaxial compression experiment and simulation

3. Analysis of numerical simulation results

3.1. Thermal-mechanical coupling model

We used the calibrated meso-parameters to establish a mechanical model. On this basis, we enabled command to start the thermal module calculation. At this time, the mechanical model has been transformed into a thermodynamic model. We applied the given basic thermal parameters, boundary conditions, etc. to all particles, such as thermal expansion coefficient, specific heat capacity, thermal resistance and other thermal parameters. The thermal resistance value cannot be directly assigned to the particles. It can be programmed and calculated through the built-in FISH language of the PFC. The thermal conductivity was used to obtain the thermal resistance value, and the FISH language was used to apply a temperature field to the model. Table 3 shows the thermal parameters of the model. The thermal conductivity was calculated by fitting the temperature change curve of the sample at different temperatures.

Table 3 Thermal parameters of the model

| Thermal expansion coefficient/1·$k^{-1}$ | Specific heat capacity /J $(kg \cdot k)^{-1}$ | Thermal Conductivity/W $(m \cdot k)^{-1}$ |
|----------------------------------------|--------------------------------|------------------------------------------|
| $1 \times 10^{-4}$                     | 800                          | 4.14                                     |

The simulation operation process is as follows: After the mechanical model was established, the walls were built at the upper and lower ends of the model, and the thermal resistance between the wall and the particles was set to infinity. Then the model added a temperature field. Since the temperature of the wall was fixed and immutable, the particles in contact with the bottom wall were used as the heat source, and different temperatures (150°C/200°C/250°C/300°C/350°C/400°C/450°C/500°C/550°C/600°C), the initial temperature of all particles was 20°C, and the temperature of the heat source particles was set to rise to the rated temperature in a short time. The heat calculation time adopted solve thermal time 7200, which corresponded to the actual test time 7200s. Fig.5 is a thermal model diagram. The size of the model was 50mm×100mm. We recorded the temperature change curve of the particles with the same height at the 5 measuring points during the test as the temperature curve of the model. The heights were 10mm, 30mm, 50mm, 70mm and 90mm, which were the central particles of the shadow circles at 5 different positions in the figure.
3.2. Unidirectional heating test and simulation

Fig. 6 shows the relationship between wall stress, temperature and operating time steps of the 450℃-600℃ model. The thermal stress and the temperature change of the measuring point during the simulation were monitored, and compared with the test results, it was found that except for temperature measuring point 3, and the temperature of other measuring points and the thermal stress curve were very similar, indicating that the simulation was more accurate.

Fig. 7 is the temperature cloud diagram of the model at different heating times at 600℃. It can be seen that as the particle temperature increased, the model began to expand.
3.3. Variation law of model thermal strain

The green particles in the model were the heat source particles, and the red and light blue particles were the particles near the middle area on the left and right sides respectively, based on the x and y coordinates. The purpose of grouping was to calculate the average value of the x-coordinates of the particles on both sides, and used the difference of coordinate changes to calculate the lateral strain of the model, that was, the model thermal strain, as shown in Fig.8.

It can be seen from Fig.8 that as the heating temperature of the model increased, the thermal strain also increased linearly. However, when the heating temperature was 450°C and 600°C, the thermal strain was obviously improved compared with the previous one, reflecting the at 450°C and 600°C, large changes occurred inside the model. The authors believed that when the heating temperature of the thermal model was low (150°C-400°C), the thermal strain of the model changes little; once the temperature reached 450°C, larger-scale cracks were formed inside the model, and the thermal strain increased; the temperature continued to increase, reaching 600°C, which was the second threshold. Large-scale cracks expanded or new larger-scale cracks were formed, resulting in a further increase in thermal strain.

3.4. Crack distribution law

Fig.9 shows the crack distribution of the model at different temperatures. The yellow is the shear crack and the green is the tensile crack. After 250°C, the distribution of cracks had a great similarity. In the process of unidirectional heating, shear cracks were dominant. This was because the upper and lower ends of the rock model were fixed. After being subjected to heat conduction, the model had a tendency to expand laterally, so when the lateral stress exceeded the shear strength of the particle bonding, shear failure would occur; when the temperature was low, the scale of the cracks was small and aggregates on the outside of the model, when the temperature gradually increased, the cracks aggregated and penetrated, forming the main crack.
4. Conclusions

(1) By using commands to monitor the wall stress and the changes in temperature measurement points, the relationship between the model thermal stress, the temperature at different heights of the model and the running time was obtained. It is found that the data obtained from the experiment and simulation were similar. It is indicating that the simulation results were more accurate.

(2) As the simulated temperature increased, the axial thermal strain would also increase, and the thermal strain increased suddenly at 450℃ and 600℃. It can be seen that 450℃ and 600℃ were the temperature thresholds. When the model was at these two temperatures, large-scale cracks were formed inside and a second large-scale crack evolution occurred.

(3) By comparing the crack diagrams after the operation at different temperatures, it is found that the number of cracks in the model increased with the increase in temperature, and the shear cracks were mainly shear cracks, indicating that the models would expand laterally under the action of thermal stress, and the failure form of the model was mainly shear failure.

Acknowledgment

This study was financially supported by the Shandong Natural Science Foundation (No. ZR2020ME084), the National Natural Science Foundation of China (No. 51504142), the Qingchuang Science and Technology Program of Shandong Province University (No. 2019KJG008), the Scientific Research Foundation of Shandong University of Science and Technology for Recruited Talents (No. 2017RCJ013), the SDUST Research Fund (No. 2018TDJH102), and the Geological Survey Project of China Geological Survey (No. 447 DD20190182).

References

[1] Wiatowski M, Kapusta K. Evolution of tar compounds in raw gas from a pilot-scale underground coal gasification (UCG) trial at Wieczorek mine in Poland. Fuel 2020;276:118070.
[2] Xin L, Li C, Liu W, Xu M, Xie J, Han L, et al. Change of sandstone microstructure and mineral transformation nearby UCG channel. Fuel Processing Technology 2021;211:106575.
[3] Xu M, Xin L, Liu W, Hu X, Cheng W, Li C, et al. Study on the physical properties of coal pyrolysis in underground coal gasification channel. Powder Technology 2020;376:573-592.
[4] Xu ZY. Effect of heterogeneity of brittle rock on fracture mechanism under thermal-mechanical coupling effect. Chengdu: Chengdu University of Technology, 2014.
[5] Wu Z, Zhou Y, Fan L. A fracture aperture dependent thermal-cohesive coupled model for modelling thermal conduction in fractured rock mass. Computers and Geotechnics 2019;114:103108.
[6] Huang YH, Yang SQ, Bu YS. Effect of thermal shock on the strength and fracture behavior of pre-flawed granite specimens under uniaxial compression. Theoretical and Applied Fracture Mechanics 2020;106:102474.
[7] Ali AY, Bradshaw SM. Bonded-particle modelling of microwave-induced damage in ore particles. Minerals Engineering 2010;23:780-790.
[8] Zhai C, Sun K M, Li K. Hot dry rock coupling damage model of thermalhydrological-mechanical and its research of numerical simulation. Journal of Wuhan University of Technology 2010;32:65-69.

[9] Li ZY. Study on the Breaking Law of High Temperature Rock under Ultrasonic. Jilin: Jilin University, 2020.