A Thermal-Hydrological-Mechanical-Chemical Coupled Mathematical Model for Underground Coal Gasification with Random Fractures

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Abstract: In this paper, in order to understand the development process and influencing factors of coal underground gasification, taking the two-dimensional underground gasification area of the plane as the simulation object, the characteristics of the multi-physical field coupling process of exudate mass heat transfer and combustion gasification reaction in the process of horizontal coal seam underground gasification are analyzed, and a two-dimensional mathematical model of thermal-hydrological-mechanical-chemical coupling of a porous medium is established. The temperature distribution of coal rock from the gasification point, the distribution of gas water vapor pressure and stress-strain, the temperature contour distribution of fractured coal rocks of different densities of heterogeneity, and the influence of different water-oxygen ratios and different fractured coal rocks on the gas components generated by the gasification reaction were studied. The results show that the tensile damage caused by the tensile strain volume expansion of the coal underground gasification center, the shear damage caused by the compression of the edge compressive strain volume, and the temperature conduction rate decrease with the increase in the coal rock fracture, but in the heterogeneous coal rock, the greater the fracture density, the faster the temperature conduction rate, which has a certain impact on the gasification combustion reaction. The ratio of CO, H2 and CO in the case of simulating that the water-to-oxygen ratio is 1:2, 1:1, and 2:1 is 1:0.85:0.73, 1:1:0.97, and 1:1:0.6:1.33, respectively. At a water-oxygen ratio of 2:1, the concentration ratio is the most ideal, and the main gases, CO, CO2, and H2 are 32%, 21%, and 37%. Furthermore, the reaction rate increases with the increase of fracture density. The gas component concentration simulated in this paper has good consistency with the results of the previous experimental data, which has important guiding significance for the underground coal gasification project.

Keywords: underground coal gasification; multi-physical field coupling; different fissure coal rocks; gas composition

MSC: 74A45; 74E35; 74F05; 74F25; 74L10; 74S05; 80A19

1. Introduction

Coal underground gasification technology is a method of chemical mining to directly burn coal in situ to produce combustible gases, which integrates the three major processes of well building, coal mining and gasification and has the advantages of good safety, less investment, high efficiency and less pollution [1,2]. Since the last century, underground coal gasification has been of wide interest in the world and has been applied to a number of underground gasification industrial tests at home and abroad, which is suitable for in situ mining and gasification of non-minable coal seams, low-grade coal seams and deep
coal seams [3,4]. The technology improves the utilization rate and industrial value of coal, reduces the direct emission of greenhouse gases to the atmosphere, and has broad application prospects [5-7].

Although underground coal gasification has advantages for the environment and good economic benefits, due to the invisibility and complexity of coal underground gasification, there are many problems in the gasification process, such as the stability of the surrounding rock of the gasification channel [8,9]. With the expansion of the coal underground gasification stope, the top bottom slate layer near the gasification channel is subjected to high-temperature thermal stress, its own gravity, structural stress, gas pore pressure and other joint actions to produce a large number of cracks. When the gasification area reaches a certain scale, the top slate layer moves and collapses, resulting in the overlying rock fissure penetration and groundwater or surface water immersion into the furnace. When serious, this can extinguish the combustion area and, at the same time, cause gas leakages, overflow and other issues [10]. More importantly, the purpose of underground coal gasification is to obtain better gas components, and problems such as surrounding rock damage in the gasification process will cause gas calorific values and concentrations to decrease. Therefore, in order to evaluate the stability of the gasification surrounding rock and the economy of the gas component, scholars at home and abroad have carried out a large number of experimental studies and numerical simulations on the stress damage and gasification reaction of high-temperature coal rocks [11]. In the study of factors influencing the concentration of gas components, Cui et al. [12] established a two-dimensional mathematical model coupled with the non-steady seepage transport and chemical reaction of porous media and studied the movement speed of the flame working surface, the temperature field of the combustion zone and the gasification zone. Perkins et al. [13] established a model of heat and mass transport, commenting on migration phenomena in seepage beds and the carbon ash and pore space of chemical reactions. Wiatkowski et al. [14] used the shaft method to conduct underground coal gasification experiments and found that the gasification efficiency of shallowly buried coal seams and the risk of gas leakage were very large. Li et al. [8] studied the influence of coal species on the motion characteristics of the overlying formation and surface combustion space area. Wu et al. [15] established the thermo-hydraulic-chemical model for the dynamic behavior of UCG reactors and studied temperature development, syngas composition, pore structure alteration of coal, and cavity growth pertinent to the UCG process. The above scholars studied the final gas component concentration by using temperature and gas flow as the main factors affecting the gasification reaction. In the study of factors affecting stress damage in surrounding rocks, Lu et al. [16] conducted thermo-physical property experiments at high temperatures, studied the thermo-mechanical coupling of overburden in the combustion air zone, and obtained the temperature distribution map and tensile damage distribution law of the gasification of the surrounding rock. Huang et al. [17] studied the temperature field, stress field and displacement field of the surrounding rock in the hollow combustion area of coal underground gasification strip mining and obtained the stress distribution and displacement deformation law of the top and bottom plate. Mehdi et al. [18] used Flac3d simulation software to establish a model to predict the stress distribution of coal rock layers during the underground gasification process of coal and proposed a stability analysis method for a coal underground gasification coal column on the basis of the model. Mojtaba et al. [19] conducted three-dimensional simulations of heat, mass transfer phenomena and chemical kinetics during coal seam combustion and studied the gas component flow, cavity shape and temperature distribution during coal seam gasification. These scholars used temperature and gas flow as the main influencing factors to study the distribution of stress damage in the surrounding rock.

At present, the research on the underground gasification of coal is mainly to ensure the stability of the surrounding rock on the gasification channel to ensure the safety of the underground gasification working surface; the other purpose is to explore the concentration of the gas produced in the gasification process and the proportion of gas components...
to ensure the economy of the gasification work [20]. The heterogeneity and anisotropy of the physical and mechanical properties of the surrounding rock have a great influence on the thermal fracture of high-temperature rock formations [21]. Temperature heat transfer is not only related to the thermal conductivity of rocks but also has a coupling relationship with the seepage of gas in pore fractures in rock formations [22,23]. Due to the limitations of the physics applied by previous scholars to the problem of underground coal gasification and the relatively single material model, the inter-coupling factors in many physics are not really considered and can easily bring errors to the final results. Based on this, this paper takes into account the main physics changes in the process of coal underground gasification and combines multi-field coupled finite element software to simulate the real coal underground gasification environment characteristics. Specifically, using the method of thermal-hydrological-mechanical-numerical simulation combined with the principle of simple chemical reactions, establishing heterogeneous rock models with random fractures, the temperature, stress damage and gas composition coupled to the heterogeneous surrounding rock of underground coal gasification under the conditions of unidirectional heating, constraint, gas injection and gas production are studied in order to provide a mechanism of assessment for the damage and rupture of coal underground gasification rock, gas concentration and surrounding rock stability.

2. A Thermal-Hydrological-Mechanical-Chemical Coupled Mathematical Model for Underground Coal Gasification

It is assumed that a coal seam is a porous and multiphase medium, and the mechanical properties are elastoplastic materials, which are composed of solid-phase particles, water, a small amount of water vapor and a certain pressure of free and adsorption gas [24]. The diffusion and seepage of the gas follow Fick’s law and Darcy’s law, and the moisture in the coal seam adheres to the solid particles and does not produce seepage.

2.1. Coal Seam Deformation Equation

Due to the effect of temperature expansion, the coal seam is subject to thermal expansion stress of the coal matrix and gas pressure of the pores of the coal seam [25]. We begin by establishing the non-isothermal deformation equation for the Navigator form [26]:

\[
Gu_{i,j} + \frac{G}{1-2\nu}u_{j,j,i} - \alpha(p_{f,i} + p_{v,i} + p_{p,i}) - Ke_{s,i} - K\alpha T_{i} + f_{i} = 0
\]

where \(G = \frac{E}{2(1-\nu)}\), \(K = \frac{E}{3(1-2\nu)}\), \(\alpha = 1 - \frac{K}{K_s}\), \(e_s = e_L V_{rg}\), \(G\) is the shear modulus of coal, \(K\) is the volume modulus of the coal matrix, \(K_s\) is the volume modulus of coal particles, \(E\) is the modulus of elasticity, \(\nu\) is Poisson’s ratio, \(\alpha\) is the Biot factor, \(\alpha_T\) is the coefficient of thermal expansion, \(p_f\) is the pressure of free gas in the fissure, \(p_v\) is the coal seam water vapor pressure, \(T\) is the seam temperature, \(f_i\) and \(u_i\) (\(i = x, y, z\)) is the volume force and displacement in the \(i\) direction, \(e_s\) is the volumetric strain due to gas adsorption or desorption, \(e_L\) is the adsorption strain under unlimited pore pressure, and \(V_{rg}\) is the volume of adsorbed gas per unit mass coal seam expressed in the equation by Langmuir [27]:

\[
V_{rg} = \frac{p_m}{P_L + p_m} \exp \left[ -\frac{c_2}{1 + c_1 p_m} (T - T_m) \right]
\]
where $p_m$ is the adsorbed gas pressure in the coal seam matrix, $T_{ar}$ is the critical temperature of gas adsorption and desorption, $P_L$ is the Langmuir pressure constant at $T_{ar}$ temperature, and $c_1$ and $c_2$ are pressure and temperature constants.

It is assumed that the rock satisfies the following constitutive relationships in the uniaxial stress state. It is also assumed that when the stress state in which the material is located satisfies the maximum tensile stress criterion or the Mohr–Coulomb criterion, the rock begins to exhibit tensile or shear damage, where $F_t$ and $F_c$ can be expressed as [16]

$$F_t = \sigma_1 - \sigma_{t0}$$
$$F_c = |\sigma_3| + \frac{1 + \sin \varphi}{1 - \sin \varphi} \sigma_1 - \sigma_{c0}$$

(3)

where $\sigma_1$ and $\sigma_3$ are the first main stress and the third main stress, respectively; $\sigma_{t0}$ and $\sigma_{c0}$ are the tensile and compressive strength of the rocks. $\varphi$ is the rock friction angle.

According to the constitutive relationship of the rock, the relationship between the damage variable $D$ and the strain can be defined as [16]

$$D = \begin{cases} 0 & (F_t < 0, F_c < 0) \\ 1 - \exp \left( \frac{\varepsilon_1^2}{\varepsilon_{t0}^2} \right) & (F_t \geq 0, |\varepsilon_1| \geq |\varepsilon_{t0}|) \\ 1 - \exp \left( \frac{\varepsilon_3^2}{\varepsilon_{c0}^2} \right) & (F_c \geq 0, |\varepsilon_3| \geq |\varepsilon_{c0}|) \end{cases}$$

(4)

where $\varepsilon_1$ and $\varepsilon_3$ are the first main strain and the third main strain, respectively; and $\varepsilon_{t0}$ and $\varepsilon_{c0}$ are the limits of rock elasticity under uniaxial compression, respectively. The damage variable $D(0 \leq D \leq 1)$ can represent the main damage burning area of coal rock. $D = 0$ indicates that the coal rock has not been damaged, and $D = 1$ indicates that the coal rock has been completely damaged.

### 2.2. Gas Transport Equation

The gas transport mechanism in the coal seam matrix is a diffusion-led process based on Fick’s first diffusion law, which can be expressed as the following equations for the adsorption gas transport of coal seams [28]:

$$\frac{\partial m_b}{\partial t} = -\frac{1}{\tau RT} \left( p_m - p_f \right)$$

(5)

$$m_b = \rho_s \rho_a V_L V_{sg}$$

(6)

where $m_b$ is the absorbed gas content in matrix, $M_g$ is the gas molar mass, $\tau$ is the adsorption gas desorption time, $t$ is the total time, $R$ is the universal gas constant, $\rho_s$ is the seam density, $\rho_a$ is the gas density at standard atmospheric pressure, $T_a$ is the standard temperature at standard atmospheric pressure, $V_L$ is the Langmuir volume constant at $T_{ar}$ temperature.

According to the ideal gas equation of state, any gas density can be expressed as:

$$\rho = \frac{M}{RT} p$$

(7)

We bring Equations (4) and (5) into (3) to obtain the matrix gas diffusion equation:
The transport mechanism of gases (water vapor, free gas) in coal seam fractures is a process dominated by seepage, which can be expressed based on Darcy’s law and the mass continuity equation:

\[
\nabla \cdot (\rho_f \nabla \phi_f) + \rho_f \frac{\partial \phi_f}{\partial t} + \nabla \cdot (\rho_v \nabla \phi_v) = -\frac{\partial m_w}{\partial t} + S_g^* \quad (9)
\]

\[
\nabla \cdot (\rho_v \nabla \phi_v) = \frac{\partial m_v}{\partial t} + S_v^* \quad (10)
\]

where the free gas seepage velocity is \( \vec{v}_f = \frac{k}{\mu_g} \nabla P_f \), the vapor seepage velocity is \( \vec{v}_v = \frac{k}{\mu_v} \nabla P_v \), and \( \mu_g \) and \( \mu_v \) are the dynamic viscosity of gas and water vapor, respectively.

Suppose that the rate of mass loss of the solid phase due to dehydration is proportional to the temperature growth rate,

\[
\frac{\partial m_w}{\partial t} = A_h \frac{\partial T}{\partial t}, \quad m_w \text{ indicates that the water in the coal rock changes from liquid to gaseous at high temperatures, } A_h \text{ is the evaporation coefficient of water vapor, and } S_g^* \text{ and } S_v^* \text{ indicate the amount of change in the reaction of some gas, water vapor and coal coke during the underground gasification of coal.}
\]

2.3. Chemical Reaction Processes

The chemical reaction of underground coal gasification is a complex process of change, including both homogeneous reactions and heterogeneous reactions [29,30], as well as complex flow, heat transfer and mass transfer processes of reactions to generate gases [31]. This paper assumes that the combustion reaction of coal coke gasification follows the Arrhenius equation. The main chemical reaction formula, pre-exponential factor \( A \) and apparent activation energy \( E_a \) are derived from the reference literature and their data is shown in Table 1. The reaction gas is not considered part of the heat transfer and seepage velocity, and its diffusion and flow are affected by the permeability coefficient of the gas, water vapor and solid-phase coal matrix in the coal seam. Underground coal gasification reactions are divided into drying reactions (I), pyrolysis reactions (II)-(III), and gasification reactions (IV)-(XIV). The drying range of coal is generally 20 °C–300 °C, and the pyrolysis reaction of coal begins to occur after about 300–400 °C. Due to the highest temperature of underground coal gasification reaching more than 1000 °C, the transition from drying of coal to pyrolysis reactions is very fast. There is almost no specific boundary, which can be simplified to the same reaction rate \( r_1 \) [32]. Gasification reactions are divided into solid phase and gas phase reactions, and the temperature range is about 500–1000 °C.

The coal drying reaction is as follows:

\[
C_{\text{wet}} \xrightarrow{r_1} C_{\text{dry}} + H_2O(g) \quad (I)
\]

The pyrolysis reactions are as follows:

\[
C_{\text{dry}} \xrightarrow{r_1} C + v(\text{volatiles}) \quad (II)
\]

\[
v + O_2 \xrightarrow{r_1} 1.06CO_2 + 0.729H_2O + 0.012N_2 + 0.5SO_2 + 0.03NO \quad (III)
\]

The solid phase reactions are as follows:
C + 0.5O₂ → CO (IV)
C + O₂ → CO₂ (V)
C + H₂O(g) → CO + H₂ (VI)
C + 2H₂ → CH₄ (VII)
C + CO₂ → 2CO (VIII)

The gas phase reactions are as follows:

CO₂ + H₂ → CO + H₂O(g) (IX)
CO + H₂O → CO₂ + H₂ (X)
2CO + O₂ → 2CO₂ (XI)
2H₂ + O₂ → 2H₂O (XII)
CH₄ + 2O₂ → CO₂ + 2H₂O (XIII)
CH₄ + H₂O → CO + 3H₂ (XIV)

The gasification kinetics process is defined by the equation:

\[ k = A \left( \frac{T}{T_{ref}} \right)^\alpha \exp \left( -\frac{E_a}{RT} \right) \]  

(11)

| Reaction Rate       | α  | A (1/s) | Eₐ (kJ/mol) | Reaction Enthalpy (kJ/mol) |
|---------------------|----|---------|-------------|---------------------------|
| [32,33] r₁          | 0  | 5.4 × 10³ | 78.24       | +100                      |
| [34] r₂ = k₄Co₂     | 0  | 1 × 10⁸   | 159.4       | −910                      |
| [11] r₃ = k₅Co₂     | 1  | 2.503 × 10¹⁷ | 179.4     | −393.8                   |
| [32] r₄ = k₆CO₂     | 0.5| 85.93     | 231         | +131.4                   |
| [11,32] r₅ = k₇CH₂  | 1  | 2.337 × 10⁻⁶ | 150      | −74.9                    |
| [34] r₆ = k₈CO₂     | 0.5| 0.8593    | 211         | +162.4                   |
| [33] r₇ = k₉C₄O₂C₂  | 0  | 2.75 × 10⁹ | 193         | +98.3                    |
| [32] r₈ = k₉C₄O₂C₃O | 0  | 27.8      | 12.6        | +41                      |
| [11] r₉ = k₉C₄O₂C₃O | 0  | 3.98 × 10⁹ | 167.4       | −285.1                   |
| [11,33] r₁₀ = k₉C₄O₂C₄ | -1 | 2.5 × 10¹⁸ | 167.4       | −242                     |
| [33] r₁₁ = k₁₀C₄O₃C₄H₄ | 0  | 4.4 × 10¹⁵ | 125.5       | −256                     |
| [34] r₁₂ = k₁₀C₄O₃C₄H₄ | 0  | 31.2      | 30          | −248                     |

2.4. Mixed Gaseous Species Transport Equation

The gas generated by the underground gasification reaction of coal not only diffuses freely in the coal seam but also flows by the action of water vapor and gas seepage and obtains the dilute material transfer equation [35]:

\[ \frac{\partial c_i}{\partial t} + \nabla \cdot (-\phi \vec{D} \cdot \nabla c_i) + \nabla \cdot \vec{v} \cdot c_i = \sum_{j=1}^{12} a_{ij} r_j \]  

(12)

where \( \vec{D} \) is the diffusion coefficient of the gas produced in the coal rock, \( c_i \) is the concentration of different gas components, \( i = O₂, CO, CO₂, H₂O, CH₄, H₂, N₂, SO₂, NO \); \( r_j \) is the above rate of chemical reactions, and \( a_{ij} \) is the reaction rate coefficient. For
different chemical reactions, when the gas component \( i \) is a product, then \( a_{ij} \) takes the value “+1”. When the gas component \( i \) is a reactant, then \( a_{ij} \) takes the value “−1”. When the gas component \( i \) is not involved in this chemical reaction, then \( a_{ij} \) takes the value “0”.

2.5. Energy Equations

In this paper, with reference to the self-heating reaction of coal [36], it is assumed that the pore gas and coal particles are in a state of thermal equilibrium during the underground gasification of coal. Thus, the energy balance equation can be given by

\[
\frac{\partial}{\partial t}\left[(\rho C_p)_{\text{eff}} T\right] + \rho_i C_{p,i} \vec{v}_i \cdot \nabla T + \rho_s C_{p,s} \vec{v} \cdot \nabla T - \nabla \cdot (\kappa_{\text{eff}} \nabla T) = (1-\phi)Q_{\text{heat}} \tag{13}
\]

The equivalent specific heat capacity is as follows:

\[
(\rho C_p)_{\text{eff}} = (1-\phi)\rho_s C_{p,s} + x_f \phi \rho_f C_{p,f} + x_v \phi \rho_v C_{p,v} \tag{14}
\]

The equivalent thermal conductivity is as follows:

\[
\kappa_{\text{eff}} = (1-\phi)\kappa_s + x_f \phi \kappa_f + x_v \phi \kappa_v \tag{15}
\]

The heat source for chemical reactions is as follows:

\[
Q_{\text{heat}} = \sum_i -Q_{Hi} r_i \tag{16}
\]

where \( C_{ps}, C_{pf} \) and \( C_{pv} \) are the specific heat capacity of the solid phase, gas and water vapor of the coal seam. \( \kappa_s, \kappa_f \) and \( \kappa_v \) are the thermal conductivity of the solid phase, gas and water vapor of the coal seam. \( x_f \) and \( x_v \) are the sub-coefficient of gas and water vapor, respectively. \( x_f = \frac{p_f M_f}{p_f M_f + p_v M_v}, \quad x_v = \frac{p_v M_v}{p_f M_f + p_v M_v}. \) \( M_f \) and \( M_v \) are the molar masses of gas and water vapor. \( Q_{Hi} \) is the enthalpy of reaction for each chemical reaction.

We integrate the above equations into the following:

\[
(\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} + \rho_i C_{p,i} \vec{v}_i \cdot \nabla T + \rho_s C_{p,s} \vec{v} \cdot \nabla T + (x_f \frac{M_f p_f}{p_f M_f + p_v M_v} C_{p,f} + x_v \frac{M_v p_v}{p_f M_f + p_v M_v} C_{p,v} - T \rho_s C_{p,s}) \frac{\partial \phi}{\partial t} \tag{17}
\]

\[
+ \phi C_{p,f} x_f \frac{M_f}{R} \frac{\partial p_f}{\partial t} + \phi C_{p,v} x_v \frac{M_v}{R} \frac{\partial p_v}{\partial t} - \kappa_{\text{eff}} \nabla^2 T + (\kappa_s - x_f \kappa_f - x_v \kappa_v) \nabla T \cdot \nabla \phi = (1-\phi)Q_{\text{heat}}
\]

2.6. Petrophysical and Mechanical Properties

The physical and mechanical properties of each mesoscopic unit in the rock layer are heterogeneous, and there are structural weakness surfaces. Compared with a homogeneous rock layer, the presence of heterogeneousness makes the internal stresses of the rock formation structure unbalanced and interact, which has a certain impact on the stability of the surrounding rock [37]. Therefore, the authors use the two-dimensional normal distribution function to heterogeneously treat the rock layer and then use the Monte Carlo method to construct a random fracture model to further increase the discreteness of the mechanical properties.

\[
f(x, y) = \left(2\pi \sigma_1 \sigma_2 \sqrt{1-\rho^2}\right)^{-1} \exp \left[-\frac{1}{2(1-\rho^2)} \left(\frac{x - \mu_x}{\sigma_1} + \frac{2\rho(x - \mu_x)(y - \mu_y)}{\sigma_1 \sigma_2} + \frac{(y - \mu_y)^2}{\sigma_2^2}\right)\right] \tag{18}
\]
where the parameters $\mu_1, \mu_2, \sigma_1, \sigma_2$ follow the mean and standard deviation of $(X, Y)$.

In the simulation of this paper, the value $\mu_1=\mu_2=1, \sigma_1=\sigma_2=0.1$ is taken to obtain the $f(x,y)$ function cloud diagram (Figure 1a) and then applied to the thermodynamic parameters of coal rock with fracture densities $m = 0.5, 0.8, 1.1$ (Table 2). For example, the elastic modulus of homogeneous rocks is $E_0 = 10$ GPa, and the elastic modulus of heterogeneous rocks treated by the normal distribution function is $E_i$ and $E_i = E_0 \times f(x,y)$. Then, we import $E_0$ and $E_i$ into the software to generate Figure 1b,c.

![Figure 1. Images of parameters generated by $f(x,y)$. (a) Normal function; (b) elastic modulus $E_0$; (c) elastic modulus $E_i$.](image)

**Table 2. Parameters of the random fracture geometry.**

| Number | Fracture Density $m$ | Towards the Mean/° | Towards Standard Deviation | Trace Length Mean/m | Trace Length Standard Deviation | Mean Gap Width/mm | Gap Width Standard Deviation |
|--------|---------------------|---------------------|---------------------------|---------------------|-------------------------------|-------------------|------------------------------|
| 1      | 0                   | -                   | -                         | -                   | -                             | -                 | -                            |
| 2      | 0.5                 | 90                  | 40                        | 1                   | 5                             | 2                 | 1                            |
| 3      | 0.8                 | 90                  | 40                        | 1                   | 5                             | 2                 | 1                            |
| 4      | 1.1                 | 90                  | 40                        | 1                   | 5                             | 2                 | 1                            |
| 5      | $\infty$           | -                   | -                         | -                   | -                             | -                 | -                            |

This paper obtains different fracture plots according to different random fracture densities $m$ in Table 2 and defines the image function as $im(x,y)$ (Figure 2). $Im(x,y) = 0$ indicates the coal matrix. $Im(x,y) = 1$ indicates the soft structural surface of the coal seam. Take rocks with a fracture density $m = 0.8$ as an example; for the thermodynamic parameters of rocks, the application is similar to $f(x,y)$, such as the elastic modulus $E_i$ of heterogeneous coal rocks (Figure 1c). After image function processing, we obtain $E_2$ and $E_2 = E_1 \times im(x,y) + 0.1$ Gpa. Since the elastic modulus of the rock cannot be 0, it is necessary to add “0.1 Gpa” to the right side of the equation for the initial porosity $\phi_0$ and permeability $k_0$ of the rock. We divide $im(x,y)$ into four intervals, as in Formula (19), and parameter images are generated by Comsol Multiphysics (Figure 3). Finally, these parameters and variables are imported into the corresponding equations for calculation.

$$\phi_0 = \begin{cases} 
0.05, & 0.8 < im(x,y) < 1 \\
0.10, & 0.6 < im(x,y) < 0.8 \\
0.15, & 0.35 < im(x,y) < 0.6 \\
0.20, & 0 < im(x,y) < 0.35 
\end{cases}$$

$$k_0 = \begin{cases} 
5 \times 10^{-17} \text{ m}^2, & 0.8 < im(x,y) < 1 \\
1 \times 10^{-16} \text{ m}^2, & 0.6 < im(x,y) < 0.8 \\
5 \times 10^{-16} \text{ m}^2, & 0.35 < im(x,y) < 0.6 \\
1 \times 10^{-15} \text{ m}^2, & 0 < im(x,y) < 0.35 
\end{cases}$$ (19)
Porosity can be defined as follows [26]:

\[
\phi = \alpha - (\alpha - \phi_0) \exp(S_0 - S) + A_\phi(T - T_{h0})
\]  

(20)

For ease of calculation, the porosity is simplified to

\[
\phi = \phi_0 + (\alpha - \phi_0)(S - S_0) + A_\phi(T - T_{h0})
\]  

(21)

where

\[
S = \varepsilon_\alpha + \frac{P_f}{K_s} + \frac{P_v}{K_v} - \alpha T - \varepsilon_v, S_0 = \varepsilon_{v0} + \frac{P_f}{K_s} + \frac{P_v}{K_v} - \alpha T_0 - \varepsilon_{v0}
\]

volumetric strain is

\[
\varepsilon_v = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}, A_\phi \text{ is the pore increase factor of moisture volatilization,}
\]

and \(T_{h0}\) is the critical temperature of water evaporation.
\[
\frac{\partial \phi}{\partial t} = (\alpha - \phi_0) \times \left\{ \frac{\partial \varepsilon_{\text{st}}}{\partial t} + \frac{1}{K_v} \frac{\partial p_{\text{f}}}{\partial t} + \frac{1}{K_v} \frac{\partial p_v}{\partial t} - \left[ \frac{P_t}{p_m(P_t + p_m)} + \frac{c_{2}c_{3}(T - T_m)}{(1 + c_{1}p_m)^2} \right] \varepsilon_{\text{st}} \frac{\partial p_m}{\partial t} \right\}
\]

(22)

Permeability can be defined as:

\[
k = k_0 \left( \frac{\phi}{\phi_0} \right)^3 = k_0 \left\{ \phi_0 \left( \frac{\alpha - \phi_0}{\phi_0} \right)(S - S_p) + A_y (T - T_0) \right\}^3
\]

(23)

2.7. Cross-Coupling Equations

The coal seam deformation equation is as follows:

\[
G u_{i,j} + \frac{G}{1 - 2v} u_{i,i,j} - \alpha p_{f,j} - \frac{1}{K_v} \frac{\partial p_{f}}{\partial t} - \left[ \frac{P_t}{p_m(P_t + p_m)} + \frac{c_{2}c_{3}(T - T_m)}{(1 + c_{1}p_m)^2} \right] \varepsilon_{\text{st}} \frac{\partial p_m}{\partial t} + \frac{c_{2}c_{3}V_{\text{st}}}{1 + c_{1}p_m} KT_f + f_i = 0
\]

(24)

The free gas transport equation is as follows:

\[
\nabla \left( -p_{f} \frac{\partial \varepsilon_{\text{st}}}{\partial t} \right) = \frac{1}{\tau} (p_{m} - p_{f}) - \frac{1}{\tau} \frac{\partial \varepsilon_{\text{st}}}{\partial t} + \left( \frac{\phi}{T} - (\alpha - \phi_0) \right) \frac{\partial T}{\partial t} - \left( \frac{\phi}{T} - (\alpha - \phi_0) \right) \frac{\partial T}{\partial t}
\]

(25)

The water vapor transport equation is as follows:

\[
\nabla \left( -p_{v} \frac{\partial \varepsilon_{\text{st}}}{\partial t} \right) = -(\alpha - \phi_0) p_{v} + S_{v} + \left( \frac{\phi}{T} - (\alpha - \phi_0) \right) p_{v} \frac{\partial \varepsilon_{\text{st}}}{\partial t} - \left( \frac{\phi}{T} - (\alpha - \phi_0) \right) \frac{\partial T}{\partial t}
\]

(26)

The energy equations are as follows:

\[
\frac{(\rho C_p)_{\text{eff}}}{\rho C_p} \frac{\partial T}{\partial t} + \frac{1}{K_v} \left( x_{f} \frac{M_{P} R}{x_{f}} C_{Pf} + x_{v} \frac{M_{P} R}{x_{v}} C_{Pv} - T \rho_{c} C_{Pc} \right) \left( \alpha - \phi_{0} \right) \frac{\partial \varepsilon_{\text{st}}}{\partial t} + \frac{c_{2}c_{3}V_{\text{st}}}{1 + c_{1}p_{m}} \varepsilon_{\text{st}} \frac{\partial p_{m}}{\partial t} + \frac{\phi C_{Pf}}{K_v} \left( x_{f} \frac{M_{P} R}{x_{f}} C_{Pf} + x_{v} \frac{M_{P} R}{x_{v}} C_{Pv} - T \rho_{c} C_{Pc} \right) \left( \alpha - \phi_{0} \right) \frac{\partial \varepsilon_{\text{st}}}{\partial t} = \frac{1}{K_v} \left( x_{f} \frac{M_{P} R}{x_{f}} C_{Pf} + x_{v} \frac{M_{P} R}{x_{v}} C_{Pv} - T \rho_{c} C_{Pc} \right) \left( \alpha - \phi_{0} \right) \frac{\partial \varepsilon_{\text{st}}}{\partial t} + \left( \frac{\phi}{T} - (\alpha - \phi_0) \right) \frac{\partial \varepsilon_{\text{st}}}{\partial t} - \left( \frac{\phi}{T} - (\alpha - \phi_0) \right) \frac{\partial T}{\partial t}
\]

(27)

3. Numerical Analysis of Thermal-Hydrological-Mechanical-Chemical Coupling Process of Coal Gasification

3.1. Establishment of Geometric Model

The underground coal gasification process is shown in Figure 4. This process involves injecting O_2 air and steam from the injection well, and the gas generated by the
extraction of the gas from the gas production well and its temperature, fluid flow, chemical reaction and damage affect each other [38,39]. Therefore, with reference to the coal underground gasification process diagram, a 10 m × 10 m coal rock two-dimensional geometry (Figure 5) is established in Comsol Multiphysics, and a circle with a diameter of 0.02 m is set in the geometric center as the ignition point and the injection point of the gasifier. The model is set up as gas production around the model, and the total duration of the entire process is 1 × 10^7 s. In order to simulate the multi-physics coupling process of coal subsurface gasification, Equations (8) and (25)–(27) are substituted into the PDE module. Equation (24) is substituted into the solid mechanics module. Chemical reaction formulas (I)–(XIV) are substituted for chemical reaction engineering module calculation. Equation (12) is substituted into the porous medium dilute matter transport module for coupling calculations, where the initial conditions and boundary conditions of each physics are described in Table 3, and finally, im(x,y) and f(x,y) are drawn. The function image processes and calculates thermodynamic parameters and variables such as porosity and permeability, and the resulting cloud map can be obtained.

Figure 4. Coal underground gasification flow chart.

Figure 5. Coal seam mesh model.
Table 3. Boundary and initial conditions for numerical models.

| Defined Conditions | Coal Seam Deformation | Water Vapor, Gas | Temperature Transfer Heat | Gas Diffusion |
|--------------------|----------------------|-----------------|---------------------------|---------------|
| Initial conditions | \( U_x = U_y = 0 \) | \( p_{vo} = 1 \text{ MPa}, p_0 = 2 \text{ MPa} \) | \( T_0 = 300 \text{ K} \) | \( CO_2(0) = 10 \text{ mol/m}^3 \) |
| Boundary conditions | \( U_x = 0 \) | \( p = 1 \text{ atm} \) | Thermal insulation | outflow |
| AB                 | \( U_x = 0 \) | \( p = 1 \text{ atm} \) | Thermal insulation | outflow |
| AC                 | \( U_x = 0 \) | \( p = 1 \text{ atm} \) | Thermal insulation | outflow |
| CD                 | \( U_x = 0 \) | \( p = 1 \text{ atm} \) | Thermal insulation | outflow |
| BD                 | \( U_x = 0 \) | \( p = 1 \text{ atm} \) | Thermal insulation | outflow |
| Boundary E         | Free displacement | \( No flux \) | \( T = 1273.13 \text{ K} \) | \( CO_2 = 20 \text{ mol/m}^3 \) |

3.2. The Relationship between Coal Rock Mechanics and Temperature

The mechanical properties of coal rock are as follows [40,41]:

1. Elastic modulus (GPa): \( E / E_o = 0.0361 + 1.0875/(1+\exp((T-275.1833)/53.7292)), \)
293 K \( \leq T \leq 1173 \text{ K} \)

2. Tensile strength (MPa): \( \sigma / \sigma_o = 0.1315 + 1.0739/(1+\exp(T-291.9924)), \)
293 K \( \leq T \leq 873 \text{ K} \)

3. Coefficient of thermal expansion (1/K): \( \alpha / \alpha_o = 1.2645 \exp(-T/604.3882)-0.1542, \)
293 K \( \leq T \leq 1273 \text{ K} \)

4. Poisson's ratio: \( \nu / \nu_o = 1.27914-0.27161/(1+\exp((T-307.54786)/15.61218)), \)
293 K \( \leq T \leq 1073 \text{ K} \)

5. Specific heat capacity: \( C_p / C_{po} = 2.696-1.672/(1+\exp((T-261.2368)/36.1994)), \)
293 K \( \leq T \leq 1273 \text{ K} \)

6. Thermal conductivity: \( \kappa / \kappa_o = 0.3422 \exp(T/268.1831)+0.1806, \)
293 K \( \leq T \leq 1273 \text{ K} \)

3.3. Temperature Analysis of Fractured Rocks of Different Densities

In the coal underground gasification project, due to the heterogeneity of the physical and mechanical properties of the rock layer, the temperature is not transmitted outward in the form of concentric circles, and the temperature rise rate at different domain points is uneven. In this paper, the model is calculated according to the division of the fracture plot in Figure 2, and a temperature distribution cloud map is obtained. It can be seen from Figure 6 that as the density of the fissure continues to increase, the lower the minimum temperature of its edge, which is 730 K, 680 K, 640 K, 560 K and 550 K, respectively. This is due to the fact that the conduction of temperature is composed of a form of heat conduction in which solid particles of coal rock work together with the gas in the pore, a form of thermal convection of the pressure gradient flow of gas in the fracture of coal rock, and a form of thermal radiation in parts. In general, the heat transfer of coal gasification is dominated by heat transfer. Therefore, since the thermal conductivity of the gas is much
smaller than the thermal conductivity of the solid, the increase in the fracture density is negatively correlated with the temperature increase rate. When comparing the law of temperature increase at the distance gasification point in the five fracture models, the temperature conduction is related to the proportion of solid particles, but the temperature change of rock fracture density $m = 0.5$ and $m = 0$ has almost no difference, and $m = 1.1$ is even higher than the temperature of $m = 0.8$. This is due to the fact that when there is a heterogeneous fracture in the coal rock mass, the influence of gas flow is significant, and the heat conduction increases first and then decreases with the increase in fracture density.

For the gasification of a coal seam, it is necessary to study the pore structure of the coal, simulate the conduction distribution of temperature, and then determine the gasification rate of the coal gasification working surface. Similarly, the different structures of the surrounding rocks in the combustion area will also affect the distribution of temperature and directly affect the effect of its thermal stress on the surrounding rock.

![Temperature distribution cloud diagram of different fracture densities](image)

**Figure 6.** Temperature distribution cloud diagram of different fracture densities. (a) $m = 0$; (b) $m = 0.5$; (c) $m = 0.8$; (d) $m = 1.1$; (e) $m = \infty$; (f) the relationship between temperature and distance from the gasification point.

### 3.4. Analysis of Temperature, Air Pressure, Stress-Strain and Gasification Point Distance

In this paper, the distance between temperature, adsorption-free gas pressure, and water vapor from the gasification point was studied by selecting the heterogeneous fracture density $m = 0.8$ over time. As shown in Figure 7a, the temperature change at 1 m and 2.5 m from the gasification point first increased sharply and then slowly increased. When the distance from the gasification point is 4 m, 5.5 m and 7 m, the temperature increase is almost linear. It can be seen that due to the high temperature near the gasification point, the gas pressure increases, producing a large pressure gradient and diffusing heat outward. When the temperature at the edge of the coal rock is up to about 550 K, the gas pressure gradient is small, the temperature change is mainly heat conduction and increases linearly, and the thermal conductivity increases with the increase in temperature.
Figure 7b and c show the adsorption and free gas pressure changes. It can be seen that the adsorption gas is very sensitive to temperature. The temperature is high, the pressure increases sharply to about 2.5 MPa, and then slowly desorpts out. The early pressure of the free gas pressure is almost unchanged, and the later stage is gradually reduced. This is because the free gas is also increased by the pressure of the temperature increase, but part of it reacts with the incoming oxygen to generate CO₂, and the other part seeps out. The adsorption gas is also desorbed into the fissure to replenish the free gas. Therefore, the early free gas basically maintains 2 MPa. Then, a large amount of seepage flows out and reacts to produce heat, and the gas pressure is reduced to atmospheric pressure.

The pressure of water vapor changes significantly by temperature and chemical reaction, as shown in Figure 7d. First, the higher the temperature, the higher the density of water vapor, and the more intense the expansion by heat. Secondly, when the heat of the gasification point diffuses, the water in the coal rock evaporates. Therefore, at the initial stage of 1 m closest to the gasification point, the water vapor pressure increases from the initial 1 MPa to about 2.5 MPa, and the latter part produces seepage due to the pressure gradient. The other part reacts with coal coke to generate gas. At the farthest point away from the gasification point, because the early stage is almost unaffected by temperature and chemical reactions, the water vapor seeps out. When the gasification is late, the temperature rises, and the water vapor pressure increases slightly.

Figure 7e shows the equivalence force of the coal rock mass, which generally decreases with the increase in the distance from the gasification point. However, at the farthest distance from the gasification point, that is, at 7 m, the equivalence force initially increases sharply to 4 MPa, and then continues to increase slowly. This is because when the gasification point is closest, the stress is mainly the concentrated stress of the gasification ignition air zone, the thermal stress of the high-temperature action and the gas pressure of the expansion, so the equivalent force is the largest, and the tensile damage is the most obvious. Then, farther away, the stress decreases, which can be seen in the volume strain relationship in Figure 7f. However, with increasing distance from the edge, the volume strain also decreases, which is due to the fact that the gas and water vapor at the edge at the first extracted, and the internal volume strain of the entire coal rock mass is generally increased. The edge displacement of the coal rock is affected by the normal constraint, that is, the structural stress. The volume is compressed, the volume strain is reduced, and the internal expansion of the gasified coal rock is reduced. The edge is first increased by the external constraint stress, and the stress damage change law of the coal rock can be verified by the damage cloud map in Figures 8 and 9. Therefore, tensile damage occurs at the center of the coal underground gasification coal rock by the combined effect of pore pressure and thermal stress, while the edge is mainly affected by the compressive stress of ground stress, and shear damage occurs.
Figure 7. Temperature, barometric pressure, stress-strain and gasification point distance relationship. (a) temperature $T$; (b) adsorbed gas pressure $p_m$; (c) free gas pressure $p_f$; (d) water vapor pressure $p_v$; (e) stress of von mises $\sigma_v$; (f) volumetric strain $\varepsilon_v$.

Figure 8. Coal rock tensile damage $D$. (a) $m = 0$; (b) $m = 0.5$; (c) $m = 0.8$; (d) $m = 1.1$; (e) $m = \infty$.

Figure 9. Coal rock shear damage $D$. (a) $m = 0$; (b) $m = 0.5$; (c) $m = 0.8$; (d) $m = 1.1$; (e) $m = \infty$.

The red area of $D = 1$ in Figure 8 indicates that the mechanical properties of the coal rock have completely failed, and it can be seen from (a) and (e) that the damaged area is almost axisymmetric. The area of damage and its extension of the fracture density $m = 0$ are larger, the fracture-bearing coal rock damage is uneven, and the fracture density $m = 1.1$ is the largest. Figure 9 shows the shear damage of the coal rock. The damaged area is concentrated at the edge of the coal rock, and the damaged area is much smaller than the tensile damage. The shear damage of rocks containing fissures is larger, while the edge damage of homogeneous rocks is relatively small. It can be seen that the fracture penetration and mechanical failure of the surrounding rock of coal underground gasification are mainly caused by tensile damage to the rock. Comparing the temperature map of Figure 6 with the damage $D$ of Figure 8, it is found that the temperature contour plot is similar to the damage shape, almost all of which extend outward in concentric circles. The most typical example of this can be seen in Figures 6d and 8d, where the temperature is the main factor affecting rock damage, and temperature is affected by coupling by other factors.
3.5. Coal Underground Gasification Gas Concentration Distribution

3.5.1. Proportions of Gas Products with Different Water-to-Oxygen Ratios

Figure 10a shows that when the water-to-oxygen ratio is 1:2, the CO\textsubscript{2} concentration of the underground gasification reaction of coal is the highest, reaching 33% of the whole, while the H\textsubscript{2} and CO concentrations are relatively low. The ratio of CO\textsubscript{2}, H\textsubscript{2} and CO is about 1:0.85:0.73, which is because most combustible gases and coal coke can be fully burned due to their relatively high O\textsubscript{2} concentration. In the early stage of gasification, mainly based on the reaction of coal coke and oxygen, there is also a small amount of gas and oxygen in the coal seam for combustion reactions, generating CO\textsubscript{2} and CO as well as a large amount of heat, so that the gasification working surface heats up rapidly. When the gasification working surface reacts at a constant speed, the coal seam gasification channel is mainly divided into an oxidation zone, reduction zone, and dry distillation dry zone. The oxidation zone is dominated by coal combustion heat production, but the scope is small. The temperature range of the reduction zone is about 400 °C–800 °C, and coal coke mainly reacts with hot water vapor to generate H\textsubscript{2} and CH\textsubscript{4}. H\textsubscript{2} accounts for about 28% of the gas components. The drying area of dry distillation is about 400 °C or less. The first chemical reaction of underground coal gasification is dry distillation because the composition of the coal seam mainly includes coal coke, ash, moisture, some impurities, air methane, etc. Under the action of high temperature, the first ash moisture volatilizes out, and some impurities react with oxygen to generate a small amount of NO, N\textsubscript{2} and SO\textsubscript{2}.\[\text{\textcopyright 2023 American Geophysical Union. All Rights Reserved.}\]
As shown in Figure 10b, when the water-oxygen ratio is 1:1, the CO$_2$, H$_2$, and CO concentrations are roughly equal, about 1:1:1.097. However, the concentration of CO$_2$ is reduced from the previous ratio because after the oxygen concentration is reduced, the coal coke is more likely to burn incompletely, generating more CO, and the coal coke and part of the CO$_2$ will also react to form some CO. As shown in Figure 10c, when the water-to-oxygen ratio is 2:1, the H$_2$ and CO concentrations are greatly increased, and the CO$_2$ concentration also drops to 21%. At this time, the underground gasification efficiency of coal is higher, and the gas composition ratio of CO$_2$, H$_2$ and CO is about 1:1.76:1.33, which is about 2:1 compared with the unsteady seepage transport simulated in documents [12,42,43]. Its H$_2$ concentration is 15% higher than the CO$_2$ concentration, and the H$_2$ concentration is inversely correlated with the incoming O$_2$ concentration, which is more consistent with the results of this analysis.

3.5.2. Variation of Gas Component Concentrations in Coal Rocks with Different Fracture Densities

In the underground coal gasification project, the concentration of the gasification gas product will also be different for the quality of coal in different regions. The main products of the gasification project are mainly CO$_2$, H$_2$, and CO, and the small number of auxiliary products are typically analyzed by SO$_2$ concentration. From Figure 11a, it can be seen that the CO$_2$ generation rate is positively correlated with the fracture density, and there is no large difference between the reaction rate in the early and late stages of gasification, mainly in the medium term; the concentration is also higher. This is due to the influence of the large fracture density. The flow rate of O$_2$ passing in is faster, the contact area with coal coke is larger, and the combustion reaction is more complete. Figure 11b,c is a comparison of the gasification to generate H$_2$ and CO concentrations, and it is not difficult to see that the gasification rate, gas concentration and CO$_2$ distribution results are roughly similar, but the difference is obviously small. Figure 11d is the SO$_2$ concentration generated by some impurities. In the early stage of gasification, it is still the coal seam gasification reaction rate with large fracture density, but from the middle stage and on, it is found that the gasification rate and gas concentration of homogeneous coal rock are slowly carried out, and the gasification reaction rate and product concentration in heterogeneous coal rock increase with the increase in fracture density.
4. Conclusions

(1) In this paper, by establishing a thermal-hydrological-mechanical-chemical model for a porous medium, the coupling law of gas and water vapor pressure and temperature distribution at the gasification point of coal rock is studied, and a cloud map of the stress-strain distribution of the entire coal rock is obtained. It is found that the coal rock gasification center is stretched and expanded by thermal stress and pore pressure, resulting in tensile damage, while the edge of coal rock is affected by confining pressure. The strain of the compressive body is reduced, mainly for shear damage, and the damage not only affects the mechanical properties of coal rock but also promotes the chemical reaction in the gasification channel. This model has important reference significance for the stress damage of the surrounding rock of coal underground gasification.

(2) Numerical simulation studies have shown that homogeneous and heterogeneous rock layers and rock layers with different fracture densities have a very obvious influence on temperature conduction and chemical reaction rate. The temperature conduction rate decreases with the increase in fracture density, and the chemical reaction rate increases with the increase in fracture density and rock formation heterogeneity.

(3) In the coal underground gasification project, both the water-oxygen ratio of the incoming water and the fracture density of the rock have a greater impact on the concentration of the gas components. The ratio of CO$_2$, H$_2$ and CO in the case of simulating that the water-to-oxygen ratio is 1:2, 1:1, 2:1 is 1:0.85:0.73, 1:1.1:0.97, 1:1.76:1.33, respectively. In the middle and late stages of gasification, the gasification rate and gas concentration of
homogeneous coal rock are slowly carried out, and the gasification reaction rate and product concentration in heterogeneous coal rock increase with the increase in fracture density. It is found that the gas components obtained in the case of the water-oxygen ratios of 1:2 and 2:1 are more ideal, so the amount of gasifier can be appropriately increased or decreased according to the actual different gasification conditions.

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**Nomenclature**

- $K$: Volume modulus of the coal matrix (GPa)
- $K_s$: Volume modulus of coal particles (GPa)
- $E$: Young’s modulus of coal matrix (GPa)
- $E_s$: Young’s modulus of coal particles (GPa)
- $\nu$: Poisson’s ratio
- $a$: Biot factor
- $\alpha_T$: Coefficient of thermal expansion (1/K)
- $p$: Gas pressure (MPa)
- $T$: Seam temperature (K)
- $T_{ar}$: Reference temperature of gas adsorption and desorption (K)
- $T_o$: Standard temperature at standard atmospheric pressure (K)
- $A_h$: Evaporation coefficient of water vapor (kg/(m$^3$·K))
- $S_{v}^*$: Amount of change in the reaction of water vapor (kg/(m$^3$·s))
- $\varepsilon_L$: Adsorption strain under unlimited pore pressure
- $\varepsilon_d$: Volumetric strain due to gas adsorption or desorption
- $\varepsilon_v$: Volumetric strain
- $u_i$: Volume displacement in $i$ direction (m)
- $\sigma_1$: Tensile strength (MPa)
- $c_1$: Pressure constant (1/MPa)
- $P_L$: Langmuir pressure constant at $T_{ar}$ temperature (MPa)
- $Q_{hi}$: Enthalpy of reactions for each chemical reaction $i$ (kJ/mol)
- $\rho_g$: Gas density at standard atmospheric pressure (kg/m$^3$)
- $\varphi$: Rock friction angle (°)
- $r_j$: Different reaction rate $j$ (mol/(m$^3$·s))
- $C_p$: Specific heat capacity (J/(kg·K))
- $k$: Permeability (m$^2$)
- $\rho_s$: Seam density (kg/m$^3$)
- $D$: Damage variable
- $x_f$: The sub-coefficient of gas
- $M_g$: Gas molar mass (kg/mol)
- $M_v$: Water vapor molar mass (kg/mol)
- $\tau$: Adsorption gas desorption time (s)
- $t$: Total time (s)
- $R$: Universal gas constant (J/(mol·K))
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