Simulation of CO$_2$ Injection into Fractured Coal Samples

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Abstract. Coal bed formation is widely considered a potential reservoir for CO$_2$ geological storage. The injection of CO$_2$ into coalbed formations is beneficial for reducing the CO$_2$ concentration in the atmosphere and enhancing the recovery of coalbed methane, which is a clean fuel. Natural coal mass is a complex system comprising fractures and matrixes. However, fluid transportation in this system is complicated, and its study is challenging. In this study, a dual-permeability model is established to investigate gas transportation and storage in the coal mass during CO$_2$ injection. Furthermore, the fluid transportation in the fracture and the matrix are studied, along with the mass transfer between them. The fully-coupled multiphysics model is solved using the finite element method. Besides, experiments on CO$_2$ injection and storage in the large fractured coal sample are performed using a special apparatus designed by the Taiyuan University of Technology (TUT). Furthermore, the results of the laboratory experiments and those of the numerical simulation are compared, and the model is confirmed to have high reliability. The simulation results demonstrate that the gas transportation in the fracture is much faster than that in the matrix. The pressure difference and the mass transfer between the fracture and the matrix are the primary causes of pressure increase in the matrix. However, there is a time delay between the change in pressure difference and the mass transfer. During the gas injection process, the evolution of permeability is obvious because of a decrease in effective stress. Furthermore, various cases are simulated to explore the influence of matrix permeability on the results. The results show that higher matrix permeability triggers more mass transfer and that it takes less time to complete CO$_2$ storage. The enhancement of coal matrix permeability can promote CO$_2$ flow rate in the coalbed mass and improve CO$_2$ injection efficiency.

1. Introduction

Global warming, which refers to an increase in the temperature of the atmosphere, has drawn increasing international concern for decades. The primary cause of the phenomenon is attributed to the emission of greenhouse gases (GHG), and CO$_2$ emission accounts for about 75% of the GHG emissions [1]. Meanwhile, geological storage is one of the suggested approaches toward reducing atmospheric CO$_2$ concentration. It involves the injection of CO$_2$ into underground formations, such as coalbeds [2]. The estimation of the CO$_2$ storage capacity of coalbeds around the world is between 220
[3] and 964 Gt [4]. Hence, coalbeds are a significant potential sink for anthropogenic CO₂ as they can accommodate 10–35 years of current fossil emissions (almost 27 Gt per year).

When investigating fluid transportation in rock mass, such as coalbeds, the rock mass is widely considered a dual media that comprises fractures and matrixes. The fracture system possesses high permeability, whereas the matrix system (also called the pore system) has high porosity but low permeability [5]. The fluid flow in coal involves two physically different but coupled migration processes. One process is fluid transportation in distributed networks of natural fractures (seepage-dominated), and the other process is fluid migration in much finer porous structures of the matrix blocks between the fractures (diffusion-dominated) [6].

The investigation of fluid migration in such microscopic and complex systems is difficult to accomplish by traditional lab experiments. Meanwhile, theoretical studies and numerical simulation modeling provide alternative options. The theoretical study of the dual-porosity system was initiated by Barenblatt et al. [7]. In their model, the fractured medium was represented by two completely overlapping continua: porous matrixes and fractures. The dual-porosity model proposed by Barenblatt was further modified by Warren and Root [8] to represent a naturally fractured reservoir using an idealized system. The system employed rectangular parallelepipeds with an orthogonally fractured network to represent the complex matrix-fracture structure. Bai et al. [9] proposed a dual-porosity/dual-permeability model to study petroleum production in oil reserves. The model employed a fixed fluid transfer rate to calculate the mass transfer between the matrix and fracture systems. The model is suitable for simulating liquid transportation in fractured reservoirs with low-permeability matrix blocks. However, gas transportation in reservoirs is different from that of liquid because of the compressibility of gas and pressure-dependent effective permeability. This situation becomes more complicated for coal [10] as gas diffusion and adsorption occur in the matrix [11] in addition to the seepage of fluid in the fracture. Wu et al. [12] developed a dual poroelastic model (coal matrix and fracture) to evaluate gas transportation in matrix and fracture systems, and the model was applied to investigate pre-mining coal seam gas extraction [13]. However, the transfer coefficient in the models mentioned above neglect the effect of gas compressibility. In addition, the models mainly focus on the discharge of natural gas (decrease in pore pressure), and there are few in-depth studies on the case involving an increase in pore pressure (e.g., CO₂ injection).

In this study, the dual-porosity/dual-permeability model is further modified to represent the primary medium (fracture) and the secondary medium (coal matrix). The fully-coupled model calculates the fluid flow, mass diffusion, and mass transfer in each node using the finite element method. When compared with traditional simulation models, the proposed model pays more attention to the gas injection process (pressure-increase process) and gas adsorption. Moreover, the results of laboratory experiments and numerical simulations are compared, and the model is confirmed to have high reliability. Furthermore, CO₂ transportation and mass transfer between the matrix and fracture systems during gas injection are further investigated.

2. Development of the Mathematical Model
Coal is a media that is composed of matrixes and fractures. As illustrated in Figure 1, the transportation path of gas in the coal can be divided into two parts: fracture and matrix [14]. The migration pattern of gas in the fracture is dominated by Darcy seepage. In the matrix, the gas transportation is more complex, and it is a combination of Darcy seepage and Fickian diffusion. Besides, there is mass transfer between the fracture and the matrix.
2. Basic assumptions

The following assumptions were made to obtain the governing equations:

1. Coal is a dual poroelastic continuous medium.
2. Coal can only be saturated with gas.
3. The gas in the fracture is in a free state.
4. The gas in the matrix is composed of free and adsorbed gas.
5. Change in porosity is ignored during the injection.
6. The free-state gas obeys the ideal gas law, and gas viscosity is constant.
7. The conditions are isothermal.

2.2 Governing equations

The gas flow in a porous medium is governed by the mass balance equation given by the following:

\[ \frac{\partial m_i}{\partial t} + \nabla \cdot (q_i) = Q_S \]  

where \( m_i \) is the gas content, \( \text{kg} \cdot \text{m}^{-3} \); \( t \) represents time, \( \text{s} \); \( q_i \) is the flux of gas flow, \( \text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1} \); and \( Q_S \) denotes the sink or source term, \( \text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1} \). In the equation, \( i = 1 \) or \( 2 \), where \( 1 \) represents the parameter in the fracture and \( 2 \) denotes the parameter in the matrix.

The gas in the fracture is in a free state, whereas the gas in the matrix is in free and absorbed states. Hence, the gas content in these two systems is defined as follows:

\[ m_1 = \varphi_1 \rho_1 \]  
\[ m_2 = \varphi_2 \rho_2 + m_{ab} \]  

where \( \varphi_i \) is the porosity of the fracture or matrix, \( i \); \( \rho_1 \) represents the density of free gas in the fracture and matrix, \( \text{kg} \cdot \text{m}^{-3} \); and \( m_{ab} \) is the quantity of absorbed gas in a unit mass coal volume, \( \text{kg} \cdot \text{m}^{-3} \).

Based on the ideal gas law, the density of free gas is defined as follows:

\[ \rho_1 = \frac{M}{RT} p_i \]  

where \( M \) is the molecular mass of gas, \( \text{mol} \cdot \text{kg}^{-1} \); \( R \) is the universal gas constant, \( \text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1} \); and \( T \) is the absolute gas temperature, \( \text{K} \).

Gas sorption follows a Langmuir isotherm [15]. According to the Langmuir isotherm equation, the quality of absorbed gas in a unit mass of coal is defined as follows:

\[ m_{ab} = \frac{p_{ga} \rho_c V_L}{(p_2 + p_L)} \]  

where \( V_L \) represents the Langmuir volume constant, \( \text{m}^3 \cdot \text{kg}^{-1} \); \( p_i \) represents the Langmuir pressure constant, Pa; \( \rho_c \) is the density of coal, \( \text{kg} \cdot \text{m}^{-3} \); and \( \rho_{ga} \) is the density of gas in the standard state, \( \text{kg} \cdot \text{m}^{-3} \).

The effect of gravity is small compared to the induced pressure gradient. Thus, the flow of gas in the fracture obeys Darcy’s law, and the seepage flux vector \( q_i \) in the fracture is given by the following:

\[ q_1 = \rho_1 v \]
\[ \mathbf{v} = -\frac{k_1}{\mu} \nabla p_1 \]  

where \( k_1 \) is the permeability of the fracture system, \( \text{m}^2 \), which is \( k_1 = 0.07055e^{-0.1566\sigma} \); \( \sigma \) denotes the effective stress, \( \text{MPa} \); and \( \mu \) is the dynamic viscosity of the gas, \( \text{Pa}\cdot\text{s} \).

Meanwhile, the transportation of gas in the matrix is a combination of Darcy seepage and Fickian diffusion. Hence, \( q_2 \) in the matrix is given by:

\[ q_2 = -\rho_2 \frac{k_2}{\mu} \nabla p_2 - D \nabla m_{ab} \]  

where \( k_2 \) is the permeability of the matrix, \( \text{m}^2 \); and \( D \) is the gas diffusion coefficient, \( \text{m}^2\cdot\text{s}^{-1} \).

Substituting (2)–(8) into (1) and ignoring the change in porosity, we obtain the following:

\[ \left[ \frac{M \varphi_1}{RT} + \rho_g \rho_c p_L \left( \frac{V_L}{p_2 + p_L} \right)^2 \right] \frac{\partial p_1}{\partial t} \nabla \cdot \left( \frac{M}{RT} p_1 \frac{k_1}{\mu} \nabla p_1 \right) = -\xi (p_1 - p_2) \]  

\[ + \nabla \cdot \left( -\frac{M}{RT} p_2 \frac{k_2}{\mu} \nabla p_2 \right) + \nabla \cdot \left( -D \rho_g \rho_c \frac{V_L}{p_2 + p_L} \nabla p_2 \right) = \xi (p_1 - p_2) \]  

In the above equations, \( \xi \) is the transfer coefficient between the matrix and the fracture [16], which is given by the following:

\[ \xi = \rho_{ex} \frac{\alpha k_2}{\mu} \]  

where \( \rho_{ex} \) is the gas density of the gas transport between the fracture and the matrix. The transportation distance is extremely short, and the pressure along the gas migration path can be considered to be continuous; hence, \( \rho_{ex} = \frac{M (p_1 + p_2)}{RT} \). Meanwhile, \( \alpha \) is a correction factor which is defined as \( \alpha = 8 \left( 3 \frac{1}{a^2} \right) \), where \( a \) is the grain length of the matrix, \( \text{m} \).

3. Reliability Analysis of the Mathematical Model
   3.1 CO2 injection experiment
   3.1.1 Experimental samples

![Figure 2. Coal sample: 100×100×200 mm.](image)

The tested coal samples were obtained from an underground depth of 300–450 m in Datong coalfield. The industrial analysis of the coal sample is presented in Table 1. The large samples were enveloped with plastic film and placed in a well-protected box to keep the coal samples in their original state. As shown in Figure 2, a large parallelepiped specimen (100×100×200 mm) was carefully processed for the CO2 injection experiment. The long axial direction of the specimen is parallel to the original coal bedding, and the direction of the gas injection is parallel to its long axis.

| Mad/% | V/% | FC/% | Ad/% | Ro | Coal type |
|-------|-----|------|------|----|-----------|
| 1.35  | 42.34 | 41.97 | 14.34 | 0.56 | Bituminous coal |
### 3.1.2 Gas injection experiment

A series of gas injection experiments were conducted to study CO\(_2\) injection and examine the reliability of the mathematical model. The experiments were performed using a specially designed device (Figure 3) that was developed by the Taiyuan University of Technology (TUT). The device injects different kinds of gas and measures the amount of geological sequestration. To avoid tensile damage on the specimen, the axial stress was always kept higher than the confining stress during the experiment, and the confining stress was always larger than the injection pressure.

![Figure 3. Sketch of the experimental device.](image)

Figure 4 shows the volume of CO\(_2\) stored in a unit mass of coal during CO\(_2\) injection under different injection pressures. The volume of gas stored in a unit mass of coal increased with an increase in gas injection pressure. Besides, when the injection pressure was low (1 or 2 MPa), the volume of the stored gas increased during the injection process. However, when the injection pressure was high (4 MPa), the volume of gas increased and then remained stable.

![Figure 4. Change in CO\(_2\) stored in a unit mass of coal with time.](image)

### 3.1.2 Reliability analysis of the simulation model

To examine the accuracy of the model, the volume of CO\(_2\) stored in a unit mass of coal with time was numerically solved and compared with the experimental results. The results of the 1- and 4-MPa injection pressures are shown in Figures 5 and 6, respectively.
Figures 5 and 6 show that the experimental results agree with those of our proposed simulation model, especially under low injection pressure. When the injection pressure was high, the simulation result was slightly lower than the experimental result after 4000 s. This was because the influence of gas absorption on permeability was neglected in our model [17]. Therefore, the proposed model is applicable for simulating gas geosequestration.

4. Description of the Numerical Simulation Model and Input Parameters

To investigate gas flux in the coal sample under CO$_2$ injection, simulation research was conducted, and the geometry of the CO$_2$ injection model is shown in Figure 7. The left surface is the injection face. The whole model has 2920 elements, and the number of degrees-of-freedom is 68962 with two pressures (fracture and matrix) at each node.

Meanwhile, boundary and initial conditions must be appropriately set in order to perform a proper simulation. Thus, different pressures were applied to the injection face, and no flow condition was applied to any other boundary. An initial pressure of 0 MPa was applied in the model. The input properties are listed in Table 2, and the values of some properties were selected from the literature.
Table 2. Properties of the simulation parameters.

| Parameter                                           | Value               |
|-----------------------------------------------------|---------------------|
| Density of coal, $\rho_c (kg/m^3)$                  | 1298                |
| Density of CO$_2$ under standard condition, $\rho_{ga} (kg/m^3)$ | 1.98                |
| Molecular mass of gas, $M (mol/kg)$                 | 0.044               |
| Viscosity of CO$_2$, $\mu (Pa\cdot s)$[12]         | $1.84 \times 10^{-5}$ |
| Gas diffusion coefficient, $D (m^2/s)$[14]          | $5.8 \times 10^{-12}$ |
| Langmuir pressure constant, $P_L (MPa)$[14]         | 2.26                |
| Langmuir volume constant, $V_L (m^3/kg)$[14]        | 0.03036             |
| porosity of fracture, $\varphi_1$                  | 0.02                |
| porosity of matrix, $\varphi_2$                    | 0.10                |
| The universal gas constant, $R (J/(mol \cdot k))$    | 8.3145              |
| The absolute gas temperature, $T (^{\circ}C)$       | 25                  |
| Permeability of matrix, $k_2 (m^2)$                 | $1 \times 10^{-19}$ |
| Grain length of the matrix, $a$ (m)                 | $1 \times 10^{-4}$  |

5. Results and Discussion

To better understand the gas flow sequence and gas transportation mechanism in the coal sample during the gas injection process, a probe was selected to extrude the simulation data. The probe was located in the middle of the geometry (0.05, 0.05, 0.1 m). In Section 5.1, pressure evolution in the fracture and matrix systems at the probe under 4-MPa injection pressure is analyzed. Furthermore, the mass transfer between the two systems is discussed in Section 5.2.

5.1 Pressure evolution

Figure 8 shows the pressure evolution within the different systems, in which the pressure increased at different rates. Because of the pressure gradient between the initial fracture and the injection pressure, there was a flow of free gas into the fracture network, thereby causing the pressure to increase. Meanwhile, the higher permeability of the fracture network caused the pressure to increase more rapidly. Subsequently, the pressure gradient between the fracture and matrix systems drove the free gas in the fracture network flow into the matrix. On the other hand, the rate of mass transfer and flow in the matrix was relatively slow when compared with that in the fracture, thereby reducing the pressure in the matrix.
5.2 Mass transfer

Figure 9. Change in mass transfer at the probe.

Figure 10. Evolution of mass transfer with the pressure difference between the fracture and the matrix.

Figure 9 shows the mass transfer at the probe during the gas injection process. The mass transfer sharply increased at the early injection stage and reached the peak at 14000 s. Afterward, it began to decrease, and the trend became slower after 400000 s. Finally, there was no mass transfer between the fracture and the matrix. Figure 10 illustrates the relationship between the evolution of mass transfer and pressure difference between the fracture and the matrix. As the injection time increased, the pressure difference and the mass transfer increased and then decreased. However, when the pressure difference reached the maximum (823837 Pa), the value of the mass transfer was 78% of the maximum value. This indicates that there was a time delay between the change in pressure difference and the mass transfer.

5.3 Distribution of fracture and permeability

During the injection process, there was a change in the permeability distribution and pressure evolution in the reservoir, as shown in Figure 11. The fracture pressure near the injection face was close to the injection pressure and the gas flow was faster in the fracture. The evolution of fracture permeability occurred because of the increase in gas pressure. As the high-pressure gas migrated into the reservoir, the permeability of the reservoir became larger. The pressure and permeability retained a uniform distribution at the final stage of gas injection.
Figure 11. Fracture pressure and permeability distribution along the central axis $y = z = 0.05$ m, $x \in [0 \text{ m}, 0.2 \text{ m}]$

5.4 Sensitivity analysis of matrix permeability

![Sensitivity analysis of matrix permeability](image)

Figure 12. Mass transfer between the fracture and the matrix at a specific point under different matrix permeabilities.

The permeability of the matrix is one of the main factors that affect gas transportation in coals. Figure 12 shows the mass transfer between the fracture and the matrix for different matrix permeabilities. Higher matrix permeability contributed to more mass transfer and shorter transfer time. This indicates that the enhancement of the matrix permeability triggers more mass transfer and that it takes less time to complete the CO$_2$ storage.

6. Conclusion

Both physical and numerical simulation experiments were conducted to analyze CO$_2$ geological sequestration in coal. The major findings are summarized as follows:

- The proposed dual-porosity/dual-permeability model effectively demonstrated the fully-coupled process of fluid flow, mass transport, adsorption, and permeability changes. The results and validation show that the proposed model can effectively simulate CO$_2$ injection and sequestration.

- The pattern of gas flow was sequential during the gas injection. The mass was triggered by the pressure difference between the fracture and the matrix, which was the primary cause of the pressure increase in the matrix. However, there was a delay in reaching the maximum pressure difference and the mass transfer rate during the gas injection.

- During the gas injection process, a change in permeability was evident because of a decrease in effective stress, and it even more than tripled in comparison with the initial system state. This promotes the flow of CO$_2$ in coal. Appropriate fracturing treatments can enhance fracture permeability and promote CO$_2$ geological sequestration.

- The permeability of the matrix was the key rate-limiting factor. The enhancement of matrix permeability guarantees mass transfer and ensures CO$_2$ geological storage at an improved rate.
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