Molecular Simulation Study on Adsorption and Diffusion Behaviors of CO$_2$/N$_2$ in Lignite

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**ABSTRACT:** Understanding the adsorption and diffusion of CO$_2$ and N$_2$ in lignite at high temperature is of great significance for fire prevention and control. Considering the influence of temperature on coal structure, molecular structure models of lignite at 298.15, 323.15, 423.15, and 523.15 K were constructed by molecular mechanics and dynamics, and grand canonical Monte Carlo molecular simulation was conducted for single-component and two-component systems under different temperatures, pressures, and gas ratios. The adsorption capacity was positively correlated with the pressure and molar ratio of CO$_2$ but negatively correlated with the temperature. The adsorption amount of CO$_2$ and N$_2$ is basically equal, both of which are at a low level. The CO$_2$ isosteric heat of adsorption (7.46–8.84 kcal/mol) varies significantly with temperature. The interaction energy is consistent with the change trend of adsorption quantity, and van der Waals energy plays a dominant role in adsorption. Injecting CO$_2$ and N$_2$ at the high temperature stage has a poor extinguishing effect, which can only dilute oxygen content and exchange heat, and the advantage of CO$_2$ will be lost. It may be more effective using liquid nitrogen which has the properties of low temperature and high specific heat capacity. The results are of great significance to improve the efficiency of fire prevention and suppression in underground coal mines.

**1. INTRODUCTION**

Carbon dioxide from the burning of fossil fuels has increased significantly over the past century. In 2018, global coal consumption grew by 1.4%, twice the average growth rate of the past decade. In China, with the increase in coal production, mine fires often occurred, and about 90% of mine fires were caused by spontaneous combustion of coal. Coal spontaneous combustion not only causes serious loss of resources, property, and life but also emits greenhouse gases. Injecting N$_2$ and CO$_2$, which are at a low level. The CO$_2$ isosteric heat of adsorption (7.46–8.84 kcal/mol) varies significantly with temperature. The interaction energy is consistent with the change trend of adsorption quantity, and van der Waals energy plays a dominant role in adsorption. Injecting CO$_2$ and N$_2$ at the high temperature stage has a poor extinguishing effect, which can only dilute oxygen content and exchange heat, and the advantage of CO$_2$ will be lost. It may be more effective using liquid nitrogen which has the properties of low temperature and high specific heat capacity. The results are of great significance to improve the efficiency of fire prevention and suppression in underground coal mines.

Injecting N$_2$ and CO$_2$, adsorbed on the surface of coal molecules, acting as a barrier to oxygen, can effectively reduce the oxygen content in the environment and the number of effective collisions between oxygen molecules and coal molecules and contribute to the CO$_2$ storage and reduction of greenhouse gases. Moreover, injecting liquid nitrogen and liquid carbon dioxide can absorb the heat generated by spontaneous combustion of coal, effectively reduce the ambient temperature, and destroy the heat storage condition of coal. Therefore, injecting N$_2$ and CO$_2$ technology has been widely used in the field of coal spontaneous combustion prevention.

When coal adsorbs the gas molecule, it will form the molecule layer on the solid surface. The higher the gas critical temperature is, the more easily the gas molecules are adsorbed. The critical temperature of CO$_2$ and N$_2$ is 304.41 and 126.19 respectively.

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thermodynamic factor and studied the properties of CO$_2$ and nitrogen can absorb more heat. In addition, the density of CO$_2$ is higher than that of air, so CO$_2$ can be kept in the middle and lower layer after injection. It can control the lower spontaneous combustion area better. However, the boiling point of nitrogen is lower than that of carbon dioxide. The temperature of liquid nitrogen under atmospheric pressure is about $−77$ K, and the general temperature of liquid carbon dioxide is about $236$ K, which needs to be stored under high pressure and low temperature. Therefore, the cooling ability of N$_2$ is much stronger than that of CO$_2$. Moreover, specific heat capacity of CO$_2$ and N$_2$ at constant pressure is $0.85$ and $1.04$ kJ/(kg·K), respectively. That is, for every $1$ K increase in the same mass at constant pressure, nitrogen can absorb more heat.

At present, relevant research studies of the adsorption properties of coal are conducted under normal temperature. Li et al. studied the adsorption behavior of CH$_4$, CO$_2$, and N$_2$ multicomponent gases in the coal molecular model using the Grand Canonical ensemble Monte Carlo (GCMC) simulation method. Wu et al. established a macromolecular coal model and carried out molecular dynamics (MD) and adsorption simulation at 298.15–318.15 K, respectively. Meng et al. conducted an experiment and simulation study on Zhaozhuang coal adsorption of gas. Gao et al. studied the adsorption characteristics of mixed gases in lignite and found that CO$_2$ in multicomponent gases had obvious competitive advantages in adsorption. Zhang et al. carried out combined MD and GCMC simulations on the transport properties of CO$_2$ in an intermediate-rank bituminous coal at a temperature of $328$ K and a range of pressures up to $25$ MPa. Based on the Wiser bituminous coal model, Zhao et al. obtained the transport diffusion coefficient from the self-diffusion coefficient via thermodynamic factor and studied the properties of CO$_2$ and CH$_4$ diffusion in coal micropores.

The abovementioned studies on the adsorption and diffusion properties of carbon dioxide and nitrogen in coal are implemented under normal temperature conditions (below 323.15 K), but the temperature in the fire zone is generally higher. Therefore, in this paper, the cell structure models of lignite under different temperature conditions (298.15–523.15 K) are built using Materials Studio 8.0 software, and the adsorption properties of CO$_2$ and N$_2$ under four temperature structures were studied. The adsorption capacity, isosteric heat of adsorption, interaction energy, and diffusion coefficient were analyzed to better understand the effect of temperature, pressure, and gas ratio on lignite adsorption performance. In addition, a new method of fire prevention is proposed, that is, at high temperature, liquid nitrogen injection gives full play to its advantages of low temperature and high specific heat capacity, reducing the temperature of coal spontaneous combustion area and dilutes oxygen. And then, CO$_2$ is injected after the temperature dropped, giving full play to its advantages of high adsorption amount as a barrier to oxygen to prevent reignition. The research results are of great significance to improve the efficiency of fire prevention and suppression in underground coal mine.

### 2. METHODOLOGY AND THEORY

#### 2.1. Molecular Models of Coal

Because the coal structure will change greatly at high temperature, the molecular model of coal at each temperature point should be established respectively. Xiao heated lignite and bituminous coal to 323.15, 423.15, and 523.15 K and established the molecular models of lignite and bituminous coal at each temperature using NMR and XPS experimental data. Because of the strong spontaneous combustion tendency of lignite, lignite coal structural units were selected in this paper. The molecular formulas of the coal sample are shown in Table 1, and the plane molecular models at different temperatures are shown in Figure 1.

#### Table 1. Molecular Formula of the Models

| samples (K) | molecular formula | molecular weight |
|------------|-------------------|------------------|
| 298.15     | C$_{206}$H$_{206}$N$_2$O$_{44}$ | 3413.88 |
| 323.15     | C$_{168}$H$_{168}$N$_2$O$_{44}$ | 3009.43 |
| 423.15     | C$_{80}$H$_{80}$N$_2$O$_{22}$ | 3151.89 |
| 523.15     | C$_{12}$H$_{12}$N$_2$O$_{10}$ | 2749.31 |

To make the energy of the model reach a stable state, Forcite module in Materials Studio 8.0 software was used to optimize the planar coal molecular model. A Dreiding force field, which is applicable to a large number of organic and biological molecules and all the main group of inorganic molecules, was used for geometry and energy optimization at the corresponding temperature. Convergence standard was ultrafine. Charge distribution was calculated using the charge balance method (QEq), and the atomic state was used to calculate electrostatic energy and van der Waals energy. In order to make the system’s total energy achieve the optimal state, the Anneal item in the Forcite module was used for annealing dynamics calculation. The initial temperature was $300$ K, and the highest temperature was $600$ K. After geometry optimization and annealing, the molecular configurations were bent and twisted, and the total energy decreased greatly. The energy changes in the optimized basic structure of coal molecules are shown in Table 2, and the basic structural units are shown in Figure 2a–d.

Five optimized coal molecular infrastructures were randomly placed into periodic crystal cell units. And then, geometry, energy, and NPT dynamics (1 ns with Nose thermostat and Berendsen barostat) optimizations were carried out on the crystal cell units to obtain a stable coal molecular model. The lattice parameters of optimal configurations are shown in Table 3. The edge length $A = B = C$; interedge angle $\alpha = \beta = \gamma = 90^\circ$. In addition, the density was close to the lignite models established by other scholars. The actual density of lignite is generally $1.1–1.2$ g/cm$^3$. This is due to the presence of small molecules in the coal structural pores and the influence of trace elements in nonmineral forms. The coal molecular models under periodic boundary conditions are shown in Figure 2e–h. The blue area is the pore structure. At the same time, the CO$_2$ and N$_2$ molecular models were constructed and their energy was optimized to achieve better results in adsorption simulations.

#### 2.2. Simulation Details

In this paper, Materials Studio 8.0 software was used to simulate coal sample adsorption of inert gas. The GCMC method was adopted to obtain the adsorption isotherms under different temperature conditions. The temperature conditions were specified as 298.15, 323.15,
423.15, and 523.15 K, respectively, and the pressure conditions were 0–10 MPa. The fugacity was converted into pressure using the Peng–Robinson formula. The Sorption module was used to perform physical adsorption on the gas under the condition of isothermal. The adsorbate molecules were treated as rigid small molecules, and the Metropolis algorithm was used to accept or reject the exchange (probability: 39%), conformer (20%), rotate (20%), translate (20%), or regrow (2%) of gaseous adsorbate molecules based on energy changes. The Dreiding force field and charge balance method (QEq) were selected. The Ewald Group method was used to calculate the electrostatic force. The atom-based

Figure 1. Molecular structure model of lignite.
method was used to calculate van der Waals forces. Also, the cutoff distance was 1.25 nm. The maximum number of simulation steps was determined to be $2 \times 10^7$, among which the equilibration steps were set as $1 \times 10^7$, and the production steps were $1 \times 10^7$. Accurate average data were obtained by sampling. In the study of binary gas adsorption, four kinds of temperature conditions were also set up. The molar ratio of CO$_2$ and N$_2$ was 0.2/0.8, 0.4/0.6, 0.6/0.4, and 0.8/0.2, and other parameters were set the same as the one-component gas adsorption.

### 3. RESULTS AND DISCUSSION

#### 3.1. Adsorption Amount and Selectivity

3.1.1. One-Component Gas System. The adsorption isotherms of single-component CO$_2$ and N$_2$ at 298.15, 323.15, 423.15, and 523.15 K are shown in Figure 3. The adsorption simulation data were fitted well using the Langmuir formula. The specific parameters are shown in Table 4. Parameter $a$ is the adsorption constant (mmol/g), indicating the maximum adsorption capacity of the adsorbent when the pressure tends to infinity at a certain temperature. Parameter $b$ is another adsorption constant (MPa$^{-1}$), and $R^2$ is the coefficient of determination.$^{13}$ It is obvious that under the same temperature and pressure, the adsorption amount of CO$_2$ is much higher than that of N$_2$, which is consistent with the previous results.$^{14,31}$ The adsorption amount of N$_2$ increased slowly with the increase in pressure, and the growth rate decreased gradually. The adsorption amount of CO$_2$ increased rapidly with pressure before 1 MPa and tended to be constant after 3 MPa. With the increase in temperature, the adsorption amount of CO$_2$ and N$_2$ decreased significantly. At 0.1 MPa, the adsorption amount of CO$_2$ and N$_2$ with temperature is shown in Figure 4. The number of CO$_2$ molecules adsorbed in the coal molecular model was significantly larger than N$_2$ molecules at 298.15 K. When the temperature reached 523.15 K, the drop of CO$_2$ adsorption amount was significantly greater than N$_2$, from 1.060 to 0.026 mmol/g, indicating that CO$_2$ adsorption was more sensitive to temperature. The adsorption amount of CO$_2$ and N$_2$ was basically equal at 523.15 K. It indicated that when inert gas was injected into the high temperature fire area, the adsorption amount of CO$_2$ and N$_2$ was relatively small, and the effect as a barrier between coal and oxygen was not effective. It was mainly by heat exchange and dilution of the oxygen concentration in the air to control the temperature of fire regions.

3.1.2. Binary Gas System. Here, the binary gas system at room temperature was discussed first. The adsorption...
isotherms and adsorption sites of CO₂ and N₂ with different gas molar ratios at 298.15 K are shown in Figure 5. The Langmuir fitting parameters are shown in Table 5. Under each gas molar ratio, the adsorption capacity of CO₂ was much larger than N₂, indicating that CO₂ had obvious competitive adsorption advantage in the binary gas system. The reason is that the adsorption capacity of the gas is positively correlated with its critical temperature. The critical temperatures of CO₂ and N₂ are 304.41 and 126.19 K, respectively, so the stronger affinity of CO₂ leads to greater adsorption amount. Therefore, it is more effective to suppress spontaneous combustion of coal with CO₂ than N₂, which is not reasonable under high temperature conditions.

The relationship between the total adsorption amount with different gas ratios and temperatures at 0.1 MPa is shown in Figure 7. Because CO₂ is more competitive and sensitive to temperature, the change in the total adsorption amount of the binary system is mainly affected by CO₂. It can be seen that the total gas adsorption amount increased with the molar ratio of CO₂/N₂ at low temperature, while above 423.15 K, the total gas adsorption amount remained at a low level, hardly affected by the molar ratio.

### 3.1.3. Adsorption Selectivity

Adsorption selectivity describes the competition degree between two components in a multicomponent mixture. Adsorption selectivity $S_{i/j}$ is defined as $S_{i/j} = \frac{x_i}{x_j}$, where $x_i$ (or $x_j$) and $y_i$ (or $y_j$), respectively,

$$\begin{align*}
\text{Table 4. Langmuir Fitting Parameters of Pure CO}_2 \text{ and N}_2 \text{ at Different Temperatures} \\
\begin{array}{|c|c|c|c|}
\hline
\text{temp (K)} & \text{CO}_2 & & \text{N}_2 & \\
\hline
298.15 & 2.557 & 3.579 & 0.939 & 1.834 & 0.306 & 0.995 \\
323.15 & 1.691 & 4.708 & 0.941 & 1.365 & 0.219 & 0.997 \\
423.15 & 1.039 & 0.519 & 0.989 & 0.848 & 0.093 & 0.997 \\
523.15 & 0.997 & 0.233 & 0.995 & 0.884 & 0.044 & 0.996 \\
\hline
\end{array}
\end{align*}$$
represent the mole fraction of i (or j) in adsorbed and free phases. The adsorption selectivity $S_{i/j}$ is greater than 1, indicating that the competitiveness of adsorbate i in the mixed component is stronger than adsorbate j. On the contrary, when $S_{i/j}$ is less than 1, it indicates that the competitive adsorption capacity of adsorbate j is stronger than adsorbate i. The higher the adsorption selectivity, the stronger the competitiveness.

The selectivity of different proportions of CO$_2$/N$_2$ at 0.1 MPa was compared, and the variation of $S_{CO_2/N_2}$ with temperature is shown in Figure 8, with the range from 6.59 to 97.06. It indicated that lignite has a higher adsorption selectivity for CO$_2$ than N$_2$ under various conditions. With the increase in the CO$_2$/N$_2$ molar ratio, the adsorption amount of CO$_2$ increased, while the adsorption amount of N$_2$ decreased. However, the ratio of CO$_2$/N$_2$ in the free phase increased more, finally leading to a gradual decrease in $S_{CO_2/N_2}$.

The adsorption selectivity showed the same trend with the temperature under different molar ratios of CO$_2$/N$_2$. That is, it first increased with temperature, then decreased rapidly at 323.15−423.15 K, and then tended to remain at about 7. The reason is that when the temperature was low, the thermal movement of gas molecules increased with temperature. Also, the chance of contact between gas molecules and adsorbents increased. CO$_2$ is more likely to preferentially occupy the adsorption site, so $S_{CO_2/N_2}$ increased first. When the temperature continued to increase, the molecular kinetic energy increased further, and the gas adsorbed on the surface of the coal matrix was desorbed out in large quantities overcoming the intermolecular forces. As a result, the adsorption amount of CO$_2$ and N$_2$ decreased significantly. In addition, CO$_2$ is more sensitive to temperature, resulting in a significant decrease in $S_{CO_2/N_2}$.

### 3.2. Isosteric Adsorption Heat

Any change in the system is accompanied by a change in energy, most of which is reflected in the form of heat. Adsorption heat refers to the direct interaction between the adsorbent and the adsorbate, and the heat is released from the adsorption process, which reflects the adsorption capacity to some extent. The average isosteric adsorption heat of CO$_2$ and N$_2$ and the standard deviations at temperatures of 298.15, 323.15, 423.15, and 523.15 K are shown in Figure 9. The isosteric adsorption heat of CO$_2$ at each temperature was about 2 times that of N$_2$, indicating that the adsorption of CO$_2$ by coal is much larger.

### Table 5. Langmuir Fitting Parameters of CO$_2$ and N$_2$ at 298.15 K

| mole ratio | a (mmol/g) | b (MPa$^{-1}$) | $R^2$ | a (mmol/g) | b (MPa$^{-1}$) | $R^2$ |
|------------|------------|---------------|-------|------------|---------------|-------|
| 0.2:0.8    | 1.860      | 2.957         | 0.926 | 0.372      | 0.491         | 0.989 |
| 0.4:0.6    | 2.086      | 5.905         | 0.970 | 0.136      | 0.908         | 0.935 |
| 0.6:0.4    | 2.178      | 7.576         | 0.947 | 0.110      | 0.283         | 0.975 |
| 0.8:0.2    | 2.215      | 7.818         | 0.926 | 0.028      | 0.793         | 0.875 |
Figure 6. Adsorption isotherms of CO₂ and N₂ at different temperatures; molar ratio of CO₂ and N₂: (a,b) = 0.2/0.8; (c,d) = 0.4/0.6; (e,f) = 0.6/0.4; and (g,h) = 0.8/0.2.
with temperature from 8.84 to 7.46 kcal/mol, which was consistent with the research results of Gao.\textsuperscript{13} It indicated that the molecular interaction between coal and CO$_2$ was gradually getting weak, corresponding to the reduction of adsorption amount in Section 3.1. The high temperature inhibited the adsorption of CO$_2$. The isosteric adsorption heat of N$_2$ slightly decreased with the temperature, which confirmed that the high temperature had little influence on the adsorption of N$_2$. However, the adsorption capacity could not be evaluated only by isosteric adsorption heat, and the comprehensive influence of pressure, temperature, gas concentration, and competitive adsorption should also be considered.

### 3.3. Interaction Energy

The interaction can reflect the stability of the system. In the system, interaction energy between the adsorbate–adsorbent molecules and adsorbate molecules includes van der Waals energy, electrostatic energy, and intramolecular energy. Because the intramolecular energy has little influence on the adsorption process, the van der Waals energy and electrostatic energy are mainly analyzed here.

The interaction energy of a CO$_2$/N$_2$ mixed adsorption system at 298.15 K increased with pressure and CO$_2$ mole fraction, as shown in Figure 10. As the pressure increased from 0.01 to 10 MPa, the interaction energy increased from $-43.359$ to $-288.104$ kcal/mol. The trend of van der Waals energy and electrostatic energy with pressure was similar. It increased rapidly in the initial stage and tended to be stable after 3 MPa, which was also consistent with the trend of adsorption amount with pressure. The greater the interaction energy is, the more likely the adsorption occurs, and the more stable the system is. Therefore, the stability of the system was enhanced with the increase in pressure and CO$_2$ mole fraction. Van der Waals energy played a dominant role in adsorption, accounting for about 70% of the total energy. According to the single-component adsorption data, the van der Waals energy between CO$_2$ and lignite was much larger than N$_2$. In addition, there was no electrostatic energy in the pure N$_2$ system, which also explained the stronger affinity between lignite and CO$_2$. As can be seen from Figure 11, the interaction energy in the system at high temperature was very small, indicating that the high temperature greatly weakened the adsorption capacity of coal to gases.

### 3.4. Diffusion Coefficient

The mean square displacement (MSD) represents the mean motion sum of molecules, as shown in eq 1. MSD can be obtained by molecular dynamics simulation. The self-diffusion coefficient is the rate of change of the mean square displacement of molecules over time, which can be calculated using Einstein diffusion\textsuperscript{34,35}, as shown in eq 2.

$$\text{MSD}(t) = \sum_{i=1}^{N} (r_i(t) - r_i(0))^2$$

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where \( N \) is the number of particles and \( \mathbf{r}_i(t) \) and \( \mathbf{r}_i(0) \) are the position vectors of molecule \( i \) at time \( t \) and 0, respectively.

First, the gas molecules were loaded into the model by a locate task according to the number of gas molecules adsorbed at different temperatures of 0.1 MPa and then the molecular dynamics (MD) simulation of the four configurations of NPT ensemble (1 ns) was carried out respectively. Subsequently, NVT ensemble (1 ns) where the volume was set such that the density matched the average density computed from the MD simulation of the four configurations of the same order of magnitude as in other literature studies, which may be caused by the coal structure expansion with the increase in temperature and the increase in gas diffusion channels. In addition, the thermal motion and fluidity of gas molecules were enhanced, which contributed to gas diffusion. After 423.15 K, the coal molecular volume shrank and the laminar structure became more compact, which led to the decrease in the gas self-diffusion coefficient. The subplot of Figure 12 illustrated that \( D_s \) was positively correlated with volume, which also proved that coal structure expansion contributed to gas diffusion.

The fractional accessible volume (FAV) of the four temperature configurations was calculated, as shown in Figure 13. The FAV represents the accessible volume fraction in the coal structure for a hard-spherical probe to pass through. In these models, the small pores (<1.5 Å) account for most of the accessible volume. Because the kinetic diameter of CO\(_2\) is 3.3 Å, the FAV of 1.7 Å probe was taken, as shown in the subplot in Figure 13. With the increase in temperature at 298.15–323.15 K, the FAV rose, and the development of pore structure of coal contributed to the diffusion of gases. As the temperature continued rising, the coal structure began to collapse and FAV decreased. Because of the increase in gas kinetic energy, \( D_s \) still rose at 323.15–423.15 K. However, the collapse of the coal structure had a greater impact on gas diffusion after 423.15 K, leading to the decline of \( D_s \).

Therefore, the effect of high temperature on the self-diffusion coefficient of CO\(_2\) in coal is mainly by changing the molecular structure of coal and kinetic energy of gas molecules.

4. CONCLUSIONS

In order to investigate the adsorption and diffusion of CO\(_2\) and N\(_2\) in lignite at high temperature, molecular structure models of lignite at 298.15, 323.15, 423.15, and 523.15 K were constructed using molecular mechanics and dynamics considering the influence of temperature on coal structure. Under the conditions of different temperatures, pressures, and gas ratios, GCMC simulation was carried out for single-component and two-component systems. Also, the adsorption isotherms obtained by simulation fitted well with the Langmuir equation. In the one-component gas adsorption system, the adsorption amount was positively correlated with pressure and negatively correlated with temperature. CO\(_2\) adsorption amount was

\[
D_s = \lim_{t \to \infty} \frac{1}{6N\Delta t} \sum_{i=1}^{N} \langle | \mathbf{r}_i(t) - \mathbf{r}_i(0) |^2 \rangle
\]
generally greater than \( N_2 \) but \( CO_2 \) was more sensitive to temperature. When the temperature reached 523.15 K, the adsorption amount of \( CO_2 \) and \( N_2 \) was basically equal, both at a low level. The relationship of adsorption amount with temperature and pressure in a binary system was basically consistent with that of a single component. Under each gas molar ratio, the adsorption sites on the surface of coal molecules were quickly occupied by \( CO_2 \), indicating the stronger affinity of \( CO_2 \). Also, the selectivity of \( CO_2/N_2 \) was negatively correlated with temperature.

The change rule of isosteric adsorption heat of \( CO_2 \) (7.46–8.84 kcal/mol) and \( N_2 \) (3.84–4.12 kcal/mol) with temperature was consistent with the adsorption amount. The change in the self-diffusion coefficient of \( CO_2 \) in coal with temperature (0.32 to 1.08 \( \times \) 10\(^{-10}\) m\(^2\)/s) was mainly affected by coal structure and molecular kinetic energy. The interaction energy (−43.359 to −288.104 kcal/mol) increased with pressure and \( CO_2 \) mole fraction, and the stability of the system was enhanced. Van der Waals energy plays a dominant role in adsorption, accounting for about 70% of the total energy. In the high temperature stage, the interaction energy and adsorption amount in the system were very small, and \( CO_2 \) and \( N_2 \) only had the effect of diluting oxygen content and heat exchange to control spontaneous combustion of coal.

Therefore, the conclusion that \( CO_2 \) is more effective than \( N_2 \) in inhibiting spontaneous combustion of coal is not reasonable at high temperature. It may be more effective to take advantage of the properties of liquid nitrogen which has lower temperature and higher specific heat capacity. That is, injecting liquid nitrogen at high temperature to absorb heat and dilute oxygen and then injecting \( CO_2 \) to be adsorbed as a barrier to oxygen, inhibit coal spontaneous combustion, and prevent reignition. The results of this study have important guiding effect on the improvement of prevention and control measures of coal spontaneous combustion.

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### Notes

The authors declare no competing financial interest.

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