Research on the Pollutant Migration Law Based on Large-Scale Three-Dimensional Similar Simulation Experiments of Underground Coal Gasification

Lin Xin,* Kaixuan Li, Mingze Feng, Weimin Cheng, Zhigang Wang, Jiaze Li, and Jing Wu

ABSTRACT: The potential pollution risk of underground coal gasification (UCG) has become a key factor restricting the development of UCG industrialization. Therefore, studying the migration and diffusion behavior of harmful pollutants is of great significance for preventing UCG pollution. In this paper, a large-scale three-dimensional similar simulation experimental device for UCG is used to simulate the gasification of Tianjin fat coal under actual working conditions. The rock layer around the simulated coal seam was sampled after the gasification was completed, the contaminants in the samples were examined by XRD, and the changes in the relative content of the contaminants at different sampling points were studied by FTIR. The results showed that benzene, phenols, aldehydes, aromatic hydrocarbons, and aromatic heterocyclic compounds remained after the gasification of No. 7 sampling point in Qianjiang, Tianjin, and that the main pollutants were aromatic hydrocarbons. The migration and enrichment of phenol and aldehyde pollutants were about the same on the east and west sides of the gasification center, while benzene pollutants were more easily migrated and enriched than aromatic heterocyclic compounds. The migration distance of phenolic pollutants on the south side of the gasification area is smaller than that of other pollutants and their maximum vertical distance from the gasification reaction area to the south is about 0.7 m. The results can provide a scientific basis for pollutant risk identification and prevention and control in the later UCG field test.

1. INTRODUCTION

According to BP’s “2016 World Energy Statistics Report”, from the perspective of global fossil energy reserves, there are abundant coal, oil, and natural gas reserves. Especially for coal resources, the current reserve-production ratio has reached 114 years. In particular, in China, the characteristics of its resource occurrence can be summarized as “rich coal, lack of oil, and less gas” in general, which determines that China’s energy structure will be dominated by coal for a long period of time. Therefore, using coal resources safely, cleanly, and efficiently has become an urgent problem to be solved. Underground coal gasification (UCG), as a coal in situ utilization technology, can not only recover and utilize low-rank coal seams that cannot be economically mined or are difficult to mine by traditional coal mining technology but can also be an effective method for mining coal seams with high sulfur, high ash, high gas, residual coal, and deep coal seam. As a result, it has received more and more attention from countries. However, an important issue that cannot be ignored is the pollution caused by UCG (Figure 1). In the process of UCG, the temperature of the oxidation zone can reach above 1100 °C and the surrounding rocks around the coal seam will produce pores and cracks under the action of high temperature and high pressure. The coal gas produced by gasification (in addition to H₂, CO, CH₄, and other combustible components, it contains benzene, naphthalene, phenol, polycyclic aromatic hydrocarbons, and other organic pollutants) may enter the aquifer through these pores and fissures to pollute groundwater. In addition, when the gasification is finished, a large amount of cooling water should be introduced into the combustion space area until the combustion space area is filled with water. At this time, the alkaline oxide in the residual coal ash after gasification is leached under groundwater immersion, increasing the pH value of water and the concentration of inorganic components (mainly harmful trace elements). However, there is still a lack of identification and evaluation of underground environmental pollutants, which has become a key factor restricting the industrialization of UCG.

Received: February 25, 2022
Accepted: April 8, 2022
Published: April 26, 2022
In this regard, many scholars have conducted a large number of theoretical and experimental studies on the pollution problems caused by the UCG technology. Li et al. took lignite as the research object and established the functional relationship between pyrolysis temperatures and pollutants by simulating the precipitation process of pollutants from UCG. Krzysztof Kapusta and others conducted a two-week onsite UCG experiment at the "Barbara" mine in Poland. They conducted extensive research on the formation, release, and migration of pollutants. Utnu et al. analyzed Malkara lignite (Turkey) and the ash generated from underground gasification and studied the composition of polycyclic aromatic hydrocarbons and their derivatives and the distribution of organic matter in the samples. Ma et al. prepared the continuous conversion product of UCG through a pyrolysis device and combined chemical analysis and thermodynamic calculation to study the chemical forms of the harmful elements in the UCG product. Ma et al. prepared the continuous conversion product of UCG through a pyrolysis device and combined chemical analysis and thermodynamic calculation to study the chemical forms of the harmful elements in the UCG product. In addition, a risk assessment code (RAC) is introduced to evaluate the risk level of harmful trace elements in the underground environment. Liu et al. used a direct drilling method to detect the combustion space of an underground borehole gasifier, studied the migration range and characteristics of the pollutants, and explored the migration path of the pollutants. Ye et al. conducted gasification experiments on Hebi bituminous coal using a two-stage method and discussed the effects of gasification products and residues on groundwater. Many scholars simulated the process of UCG through self-made experimental equipment for simulating UCG. They conducted leaching research on the residual ash and coke from gasification. Study the migration and enrichment of harmful trace elements (Hg, As, Se, Cd, Pb, Ni, Zn, etc.) leached. Sadashivam et al. conducted laboratory underground gasification simulation experiments on coal in South Wales, studied the influence of gasification pollutants under different gasification process conditions, and used some measured parameters for theoretical calculations to predict the concentration of the main balance substances in the groundwater polluted by pollutants in the UCG process. In addition, some scholars separated and extracted strains with high degradation activity toward phenol compounds from coking wastewater and domestic sewage and used the extracted strains to perform degradation experiments on gas washing water produced in the UCG model experiment to achieve the effect of pollutant degradation.

In this paper, relying on the large-scale three-dimensional similar UCG simulation device in the resource underground gasification mining laboratory, the gasification simulation experiment of Qianjiaying Coal No. 7 coal was carried out and the gasification furnace body was dissected after the furnace was closed. The samples were analyzed by sampling the simulated rock layer around the coal seam (Figure 6a) using an X-ray diffractometer and Fourier infrared spectrometer. The types of pollutants produced during the UCG of Qianjiaying No. 7 coal and their migration and enrichment in the simulated rock strata are studied to provide a scientific basis for pollutant risk identification and prevention and control in the later UCG field test.

2. MATERIALS AND METHODS

2.1. Experimental Coal Sample. The coal selected for this gasification simulation experiment is fat coal taken from the No. 7 coal of the Qianjiaying Coal Mine (Figure 2). The calorific value of raw coal (unit MJ/kg) is between 21.25 and 27.99 and the average value of medium-heat coal is 25.16 (Table 1).

2.2. Simulating Device for UCG. The simulation device for UCG (Figure 3) consists of five parts: an experimental furnace body, an air supply and exhaust system, a gas acquisition and analysis system, an automatic temperature measurement system, and an automatic temperature measurement system.

Table 1. Industrial Analysis of Coal (in percentage)\textsuperscript{a}

| $A_d$ | $V_{daf}$ | $S_d$ | $Q_{gr.ad}$ |
|-------|-----------|-------|------------|
| 27.91 | 20.83     | 0.41  | 25.16      |

\textsuperscript{a}$A_d$ = dry base ash, $V_{daf}$ = dry without ash base volatiles, $S_d$ = dry based total sulfur, $Q_{gr.ad}$ = high calorific value of coal.
and a monitoring system. Among them, the principal part is the experimental furnace body, which is a cylindrical structure with an external diameter of 3.73 m and a height of 3.54 m and is provided with a certain thickness of refractory and thermal insulation materials inside. According to the similarity theory, the experiments were conducted by laying similar materials in layers inside the furnace to simulate the rock layer around the coal seam, and monitoring devices such as thermocouples, pressure boxes, and displacement gauges were preset inside the simulated rock layer. The process gas components are detected by an online chromatograph GC-4008A dedicated to coal mines—the preset monitoring device records in real-time through a DH3818Y static stress and strain test and analysis system. DH3818Y is a static strain tester with an LCD screen, which includes three different configuration options of 8, 16, or 24 measuring channels. Each measuring channel can measure force, displacement, or strain. During measurement, functions such as sampling control and data analysis are realized through LCD screens or computer software.

2.3. Coal Seam Simulation. The simulated structure of the coal seam is shown in Figure 4a, and a 35-cm-thick similar material is laid on the bottom of the gasification furnace body to serve as the coal seam floor. A simulated coal seam with a length of 1.2 m from north to south, a width of 0.6 m from east to west, and a thickness of 0.3 m is laid with lump coal on the upper part of the bottom plate and the gaps are filled with pulverized coal. At the same time, similar materials are laid around the coal seam, and gasification channels are preset with guard pipes at the bottom of the coal seam (Figure 4). After the coal seam and similar materials around the coal seam are laid, the simulated overburden of the coal seam shall be laid layer by layer according to different material ratios, and monitoring devices such as thermocouples, pressure box, and displacement meter shall be installed.

2.4. Experimental Method. The experiment simulated the horizontal single-channel underground gasification process. A gasification channel is arranged along the coal seam floor, and the gasification agent (air, oxygen, steam, and their mixture) is injected into the south side of the channel after the commissioning of all the devices is completed. At the same time, the switch is turned on and the heating plate embedded 0.3 m from the air inlet is ignited to ignite the coal seam. Whether the ignition is successful can be judged by monitoring the temperature and gas components. After successful ignition, gasification of the simulated coal seam is carried out to study its gas production by passing gasification agents of different concentrations (Table 2). During gasification, the furnace body is in a micropositive pressure state, and the pressure in the combustion space area is about 0.05 MPa. After the gasifier is cooled, the furnace body is dissected and sampled at different locations in the combustion goaf area and similar simulated rock strata (Figure 6). A Fourier infrared spectrometer was used to analyze the functional groups of the samples, and the contaminants in the samples were characterized by XRD (Figure 5).
2.5. Samples and Analysis. 2.5.1. Sampling Situation. As shown in Figure 6a, after the simulation of the UCG experiment, samples of imitated surrounding rock around the coal seam were taken according to the interval (unit cm) and the position shown in the figure, and the samples were stored in sealed bags to prevent oxidation. Figure 6b shows the sampling situation in the gasifier after the UCG is simulated.

2.5.2. XRD Analysis. The sample was ground with an agate mortar, sieved to below 75 μm, and analyzed and tested with a high-performance, multifunctional powder crystal X-ray diffractometer (Ultima IV). Use Cu target, Kα radiation, a scan range of ~5° ~ 80°, a scan speed of 6°/min, a voltage of 20 kV, a current of 20 mA, and a step distance of 0.1° to test the organic pollutants. Using Jade 6.0 (MDI, Livermore, CA, USA) combined with the substance standard powder diffraction data (PDF) provided by the Powder Diffraction Federation International Data Center (JCPDS-ICDD), the organic pollutants are qualitatively determined according to the standard analysis method and the samples are determined by their composition of organic pollutants.

2.5.3. FTIR Analysis. An FTIR spectrum analysis was carried out using a Fourier infrared spectrometer NICOLET 380. The sample (Figure 6a) and potassium bromide (KBr) were mixed in a ratio of 1:150 and ground in an agate mortar, sieved to below 75 μm, and analyzed and tested with a high-performance, multifunctional powder crystal X-ray diffractometer (Ultima IV). Use Cu target, Kα radiation, a scan range of ~5° ~ 80°, a scan speed of 6°/min, a voltage of 20 kV, a current of 20 mA, and a step distance of 0.1° to test the organic pollutants. Using Jade 6.0 (MDI, Livermore, CA, USA) combined with the substance standard powder diffraction data (PDF) provided by the Powder Diffraction Federation International Data Center (JCPDS-ICDD), the organic pollutants are qualitatively determined according to the standard analysis method and the samples are determined by their composition of organic pollutants.

2.5.4. FTIR Data Processing. Considering that the sample's composition is relatively complex and contains a variety of functional groups, the contribution of the absorption bands of these functional groups to the infrared spectrum is relatively broad. Therefore, it is easy to generate superposition at a certain position to cause graph superposition. The amount of superposition is difficult to investigate in the absorption band of the infrared spectrum. For this reason, this paper uses the PeakFit software to determine the position and number of the initial unfolding fitting peaks according to the second derivative of the infrared spectrum. The parameters of the absorption peak are adjusted and the residual sum of squares between the original spectrum and the fitted spectrum is used as the minimum objective function as the fitting standard for fitting. In this way, the peak unfolding graph and the absorption peak parameters of the sample were obtained. Then the type of functional group was determined, and the intensity of the absorption peak was calculated.

3. RESULTS AND DISCUSSION

3.1. XRD Analysis Results. Phase identifying is also called “phase qualitative analysis”. Its basic principle is based on the following three principles: Any phase has its characteristic diffraction spectrum; the diffraction spectra of any two phases cannot be the same; and the diffraction peaks of multiphase samples are mechanical superpositions of each phase. Therefore, a “card library of known phases” is established through experimental measurement or theoretical calculation. All phases in the sample can be retrieved by comparing the spectrum of the measured sample with the “standard card” in the PDF card library.

A phase search of different sampling points found that silicon dioxide (SiO₂) and albite (Na₂O·Al₂O₃·6SiO₂) were the main phases and there was no significant change in other phases except the main phase (Figures 7 and 8). The contaminants contained in the simulated rock formations are much smaller than other substances in the simulated rock formations. Therefore, the main detection was of minor and minute phases in the phase search of organics (Figure 9). Benzene, polycyclic aromatic hydrocarbons, and some heterocyclic compounds (1,2-dicyanobenzene, 2,6-dimethylbenzoic acid, 1-naphthylamine, naphthalidionic acid, etc.) were found in 12 sampling sites. Phenolic compounds (4-octyl phenol, etc.) were found in some
sample sites. This indicates that the migration of phenolic pollutants is less than that of benzene and polycyclic aromatic hydrocarbons (PAHs).

3.2. FTIR Analysis Results. 3.2.1. Sampling and Analysis of Simulated Coal Seam Surrounding Rock. Pollutants produced by UCG are similar to surface gasification beds. Inorganic pollutants mainly include hydrogen sulfide, ammonia, and harmful trace elements of heavy metals, while organic pollutants mainly include phenols, benzene, PAHs, heterocyclic compounds, etc. In the experiment of simulating UCG, the simulated rock layer made of similar materials has a certain degree of adsorption. During gasification, the high-temperature coal gas will carry pollutants from the fissures into the surrounding rock layers and remain. For this reason, tools such as infrared spectroscopy can be used to study these pollutants at a microscopic level. Through FTIR detection of samples at sampling points, the type and relative content of the functional groups at each location can be determined to determine the contaminant migration and diffusion laws in the surrounding rock of coal seams.

Based on a large number of experiments and experiences, many scholars have summarized the types of absorption peaks in organic compounds and the assignment of their functional groups. Due to the complex composition of the samples taken, the infrared spectrograms obtained are all superimposed by combining multiple functional groups. To more clearly and accurately analyze the types of functional groups contained in the samples at the sampling points and their attributions, PeakFit and other software (the method described in Section 2.5.4) were used to perform fitting analysis on the obtained infrared spectra. By analyzing the changes of the

Figure 6. (a) Schematic diagram of the sampling of simulated rock formations around simulated coal seams and (b) simulated actual sampling of surrounding rock.

Figure 7. Smoothed XRD spectra of sampling points 1–12.

Figure 8. Sampling point No. 1.

Figure 9. 1,5 pollutant situation at the sampling point.
functional groups and their contents at each sampling point, the migration and diffusion of airborne pollutants in the surrounding rocks of the coal seam in the process of UCG are studied. Based on this, a 600–900 cm\(^{-1}\) aromatic hydrocarbon structure region and a 1000–1800 cm\(^{-1}\) oxygen-containing functional group region were selected to analyze and study the spectrogram (Figure 10).

**Figure 10.** Infrared spectrum after processing.

**Figure 11.** The fitting curve of 600–900 cm\(^{-1}\) sampling points 1–6.

**3.2.2. Different Area Analysis. 3.2.2.1. Sampling Points 1–6, 600–900 cm\(^{-1}\) Sub-Peak.** After the coal buried in the ground has undergone the process of underground gasification under different gasification agents, the harmful elements in the coal will be migrated and enriched to different degrees.\(^{33,34}\) Some of the semivolatile elements, such as cadmium, copper, zinc, etc., have relatively small changes in element concentration before and

**Figure 12.** 600–900 cm\(^{-1}\) percentage of area.

**Figure 13.** Fitting curve of 1000–1800 cm\(^{-1}\) sampling points 1–6.

**Figure 14.** 1000–1800 cm\(^{-1}\) percentage of area.
Table 3. Functional Group Attribution of 600−900 cm\(^{-1}\) at Sampling Points 1−6

| sample point | center (cm\(^{-1}\)) | area | area% | structure |
|--------------|----------------------|------|-------|-----------|
| sample point 1 | 652 | 7.173 | 7.16% | organic silicon compound Si−X stretching vibration |
| 682 | 9.510 | 9.49% | C−H bending vibration of m-disubstituted benzene |
| 709 | 13.116 | 13.08% | C−H bending vibration of monosubstituted benzene |
| 732 | 16.536 | 16.50% | aromatic heterocyclic ring stretching vibration |
| 758 | 17.439 | 17.40% | C−H bending vibration of monosubstituted benzene |
| 784 | 15.886 | 15.85% | C−H bending vibration of m-disubstituted benzene |
| 807 | 7.227 | 7.21% | aromatic heterocyclic ring stretching vibration |
| 837 | 6.089 | 6.07% | C−H bending vibration of p-disubstituted benzene |
| 870 | 7.267 | 7.25% | C−H bending vibration of pentasubstituted benzene |
| sample point 2 | 652 | 4.794 | 7.24% | organic silicon compound Si−X stretching vibration |
| 683 | 6.267 | 9.46% | C−H bending vibration of m-disubstituted benzene |
| 710 | 8.881 | 13.41% | aromatic heterocyclic ring stretching vibration |
| 733 | 10.806 | 16.32% | C−H bending vibration of monosubstituted benzene |
| 759 | 11.901 | 17.97% | C−H bending vibration of monosubstituted benzene |
| 785 | 11.901 | 17.97% | aromatic heterocyclic ring stretching vibration |
| 810 | 4.426 | 6.68% | C−H bending vibration of p-disubstituted benzene |
| 838 | 3.936 | 5.94% | C−H bending vibration of pentasubstituted benzene |
| 871 | 4.527 | 6.84% | C−H bending vibration of pentasubstituted benzene |
| sample point 3 | 648 | 3.780 | 4.46% | organic silicon compound Si−X stretching vibration |
| 672 | 7.953 | 9.38% | C−H bending vibration of benzene |
| 698 | 8.588 | 10.13% | C−H bending vibration of monosubstituted benzene |
| 721 | 11.656 | 13.75% | C−H bending vibration of m-disubstituted benzene |
| 744 | 11.545 | 13.61% | aromatic heterocyclic ring stretching vibration |
| 766 | 11.265 | 13.28% | C−H bending vibration of m-disubstituted benzene |
| 790 | 11.265 | 13.28% | aromatic heterocyclic ring stretching vibration |
| 814 | 5.258 | 6.20% | C−H bending vibration of p-disubstituted benzene |
| 841 | 6.255 | 7.38% | C−H bending vibration of pentasubstituted benzene |
| sample point 4 | 647 | 2.568 | 4.25% | organic silicon compound Si−X stretching vibration |
| 671 | 5.347 | 8.84% | C−H bending vibration of benzene |
| 693 | 5.235 | 8.65% | C−H bending vibration of monosubstituted benzene |
| 713 | 5.998 | 9.92% | C−H bending vibration of m-disubstituted benzene |
| 730 | 6.263 | 10.35% | aromatic heterocyclic ring stretching vibration |
| 748 | 6.590 | 10.76% | C−H bending vibration of monosubstituted benzene |
| 766 | 6.990 | 11.56% | aromatic heterocyclic ring stretching vibration |
| 784 | 6.709 | 11.09% | C−H bending vibration of m-disubstituted benzene |
| 802 | 4.991 | 8.25% | aromatic heterocyclic ring stretching vibration |
| 824 | 3.105 | 5.13% | aromatic heterocyclic ring stretching vibration |
| 846 | 2.853 | 4.72% | C−H bending vibration of p-disubstituted benzene |
| 872 | 3.923 | 6.49% | C−H bending vibration of p-disubstituted benzene |
| sample point 5 | 650 | 10.072 | 5.42% | organic silicon compound Si−X stretching vibration |
| 676 | 18.003 | 9.69% | C−H bending vibration of benzene |
| 705 | 22.967 | 12.36% | C−H bending vibration of monosubstituted benzene |
| 729 | 30.204 | 16.26% | aromatic heterocyclic ring stretching vibration |
| 756 | 30.996 | 16.69% | C−H bending vibration of monosubstituted benzene |
| 781 | 29.330 | 15.79% | aromatic heterocyclic ring stretching vibration |
| 806 | 16.854 | 9.07% | C−H bending vibration of p-disubstituted benzene |
| 836 | 13.233 | 7.12% | C−H bending vibration of p-disubstituted benzene |
| 870 | 14.082 | 7.58% | C−H bending vibration of pentasubstituted benzene |
| sample point 6 | 651 | 5.745 | 5.58% | organic silicon compound Si−X stretching vibration |
| 676 | 9.753 | 9.47% | C−H bending vibration of benzene |
| 703 | 12.042 | 11.69% | aromatic heterocyclic ring stretching vibration |
| 728 | 16.178 | 15.71% | C−H bending vibration of monosubstituted benzene |
| 755 | 17.316 | 16.81% | aromatic heterocyclic ring stretching vibration |
| 781 | 16.301 | 15.83% | C−H bending vibration of m-disubstituted benzene |
| 804 | 11.045 | 10.72% | aromatic heterocyclic ring stretching vibration |
| 835 | 7.237 | 7.03% | C−H bending vibration of p-disubstituted benzene |
| 869 | 7.385 | 7.17% | C−H bending vibration of pentasubstituted benzene |
Table 4. The Functional Group Attribution of 1000–1800 cm\(^{-1}\) at Sampling Points 1–6

| sample point | center (cm\(^{-1}\)) | area   | area%  | structure                                    |
|--------------|----------------------|--------|--------|----------------------------------------------|
| sample point 1 | 1031                 | 26.917 | 18.72% | C=O bond stretching vibration of ethers       |
|              | 1111                 | 23.898 | 16.62% | C=O bond stretching vibration of ethers       |
|              | 1157                 | 25.341 | 17.62% | C=O bond stretching vibration of ethers       |
|              | 1427                 | 30.485 | 21.20% | bending vibration of methyl C–H bond          |
|              | 1524                 | 13.497 | 9.39%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1564                 | 6.946  | 4.83%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1629                 | 10.224 | 7.11%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1686                 | 5.339  | 3.71%  | C=O bond stretching vibration of aldehydes    |
|              | 1744                 | 1.164  | 0.81%  | C=O bond stretching vibration of aldehydes    |
| sample point 2 | 1028                 | 18.147 | 16.96% | C=O bond stretching vibration of ethers       |
|              | 1115                 | 12.184 | 11.39% | C=O bond stretching vibration of ethers       |
|              | 1160                 | 15.062 | 14.08% | C=O bond stretching vibration of ethers       |
|              | 1366                 | 3.528  | 3.30%  | O–H bond bending vibration of phenols         |
|              | 1428                 | 20.691 | 19.34% | Bending vibration of methyl C–H bond          |
|              | 1482                 | 16.282 | 15.22% | Aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1548                 | 7.341  | 6.86%  | Aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1626                 | 9.311  | 8.70%  | Aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1696                 | 4.436  | 4.15%  | C=O bond stretching vibration of aldehydes    |
| sample point 3 | 1035                 | 6.333  | 4.55%  | C=O bond stretching vibration of ethers       |
|              | 1127                 | 18.994 | 13.64% | C=O bond stretching vibration of ethers       |
|              | 1158                 | 13.627 | 9.79%  | C=O bond stretching vibration of ethers       |
|              | 1364                 | 6.435  | 4.62%  | O–H bond bending vibration of phenols         |
|              | 1425                 | 29.403 | 21.11% | bending vibration of methyl C–H bond          |
|              | 1480                 | 25.456 | 18.28% | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1542                 | 13.649 | 9.80%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1624                 | 16.982 | 12.19% | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1695                 | 8.377  | 6.02%  | C=O bond stretching vibration of aldehydes    |
| sample point 4 | 1027                 | 21.786 | 18.80% | C=O bond stretching vibration of ethers       |
|              | 1123                 | 23.047 | 19.89% | C=O bond stretching vibration of ethers       |
|              | 1154                 | 16.555 | 14.29% | C=O bond stretching vibration of ethers       |
|              | 1379                 | 2.780  | 2.40%  | O–H bond bending vibration of phenols         |
|              | 1440                 | 27.752 | 23.95% | bending vibration of methyl C–H bond          |
|              | 1507                 | 12.164 | 10.50% | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1621                 | 9.018  | 7.78%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1695                 | 2.762  | 2.38%  | C=O bond stretching vibration of aldehydes    |
| sample point 5 | 1037                 | 10.852 | 4.14%  | C=O bond stretching vibration of ethers       |
|              | 1125                 | 35.182 | 13.41% | C=O bond stretching vibration of ethers       |
|              | 1164                 | 28.342 | 10.80% | C=O bond stretching vibration of ethers       |
|              | 1357                 | 10.440 | 3.98%  | O–H bond bending vibration of phenols         |
|              | 1416                 | 42.578 | 16.23% | C=H bond bending vibration of olefins         |
|              | 1460                 | 45.954 | 17.52% | bending vibration of methyl C–H bond          |
|              | 1506                 | 29.265 | 11.16% | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1558                 | 16.832 | 6.42%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1622                 | 24.693 | 9.41%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1682                 | 13.626 | 5.19%  | C=O bond stretching vibration of aldehydes    |
|              | 1738                 | 4.580  | 1.75%  | C=O bond stretching vibration of aldehydes    |
| sample point 6 | 1036                 | 16.338 | 10.66% | C=O bond stretching vibration of ethers       |
|              | 1117                 | 23.943 | 15.62% | C=O bond stretching vibration of ethers       |
|              | 1163                 | 21.150 | 13.80% | C=O bond stretching vibration of ethers       |
|              | 1357                 | 4.694  | 3.06%  | O–H bond bending vibration of phenols         |
|              | 1418                 | 23.580 | 15.38% | C=H bond bending vibration of olefins         |
|              | 1463                 | 21.151 | 13.80% | bending vibration of methyl C–H bond          |
|              | 1505                 | 12.678 | 8.27%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1555                 | 7.960  | 5.19%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1625                 | 14.451 | 9.43%  | aromatic hydrocarbon benzene ring skeleton vibration |
|              | 1693                 | 7.346  | 4.79%  | C=O bond stretching vibration of aldehydes    |

After gasification, while some easily volatile elements, such as mercury, will mostly migrate into the gas phase after undergoing high-temperature gasification reactions; only a small part remained in the ash. Moreover, since the raw coal undergoes complex physical and chemical changes upon underground gasification, the macromolecules in the coal easily crack to form...
Table 5. Functional Group Attribution of 600–900 cm\(^{-1}\) at Sampling Points 7–12

| sample point | center (cm\(^{-1}\)) | area | area structure |
|--------------|----------------------|------|---------------|
| sample point 7 |                     |      |               |
| 648          | 2.329                | 3.58%| Organic silicon compound Si–X stretching vibration |
| 671          | 5.223                | 8.02%| C–H bending vibration of benzene |
| 694          | 4.964                | 7.63%| C–H bending vibration of monosubstituted benzene |
| 713          | 6.714                | 10.32%| C–H bending vibration of m-disubstituted benzene |
| 730          | 6.938                | 10.66%| aromatic heterocyclic ring stretching vibration |
| 748          | 7.131                | 10.96%| C–H bending vibration of m-disubstituted benzene |
| 766          | 7.570                | 11.63%| aromatic heterocyclic ring stretching vibration |
| 785          | 7.159                | 11.00%| C–H bending vibration of m-disubstituted benzene |
| 804          | 4.815                | 7.40%| aromatic heterocyclic ring stretching vibration |
| 825          | 3.569                | 5.48%| aromatic heterocyclic ring stretching vibration |
| 846          | 3.336                | 5.13%| C–H bending vibration of p-disubstituted benzene |
| 873          | 5.339                | 8.20%| C–H bending vibration of pentasubstituted benzene |
| sample point 8 |                     |      |               |
| 648          | 3.283                | 4.57%| organic silicon compound Si–X stretching vibration |
| 672          | 5.709                | 7.95%| C–H bending vibration of benzene |
| 695          | 6.538                | 9.11%| C–H bending vibration of monosubstituted benzene |
| 717          | 9.043                | 12.59%| C–H bending vibration of m-disubstituted benzene |
| 737          | 8.837                | 12.31%| aromatic heterocyclic ring stretching vibration |
| 758          | 9.065                | 12.62%| C–H bending vibration of m-disubstituted benzene |
| 777          | 8.735                | 12.17%| C–H bending vibration of m-disubstituted benzene |
| 797          | 7.009                | 9.76%| aromatic heterocyclic ring stretching vibration |
| 820          | 3.873                | 5.39%| aromatic heterocyclic ring stretching vibration |
| 844          | 3.708                | 5.16%| C–H bending vibration of p-disubstituted benzene |
| 872          | 6.003                | 8.36%| C–H bending vibration of pentasubstituted benzene |
| sample point 9 |                     |      |               |
| 650          | 3.243                | 5.46%| organic silicon compound Si–X stretching vibration |
| 676          | 5.867                | 9.88%| C–H bending vibration of benzene |
| 705          | 7.621                | 12.84%| C–H bending vibration of monosubstituted benzene |
| 730          | 9.501                | 16.01%| aromatic heterocyclic ring stretching vibration |
| 757          | 10.018               | 16.88%| C–H bending vibration of monosubstituted benzene |
| 784          | 9.100                | 15.33%| C–H bending vibration of m-disubstituted benzene |
| 808          | 5.004                | 8.43%| aromatic heterocyclic ring stretching vibration |
| 837          | 4.392                | 7.40%| aromatic heterocyclic ring stretching vibration |
| 870          | 4.607                | 7.76%| C–H bending vibration of pentasubstituted benzene |
| sample point 10 |                   |      |               |
| 649          | 2.656                | 3.38%| organic silicon compound Si–X stretching vibration |
| 671          | 6.515                | 8.30%| C–H bending vibration of benzene |
| 694          | 5.872                | 7.48%| C–H bending vibration of monosubstituted benzene |
| 713          | 8.095                | 10.31%| C–H bending vibration of m-disubstituted benzene |
| 730          | 8.502                | 10.83%| aromatic heterocyclic ring stretching vibration |
| 748          | 8.837                | 11.26%| C–H bending vibration of m-disubstituted benzene |
| 766          | 9.680                | 12.33%| aromatic heterocyclic ring stretching vibration |
| 785          | 8.924                | 11.37%| C–H bending vibration of m-disubstituted benzene |
| 803          | 5.463                | 6.96%| aromatic heterocyclic ring stretching vibration |
| 825          | 3.788                | 4.82%| aromatic heterocyclic ring stretching vibration |
| 846          | 3.741                | 4.77%| C–H bending vibration of p-disubstituted benzene |
| 873          | 6.430                | 8.19%| C–H bending vibration of pentasubstituted benzene |
| sample point 11 |                   |      |               |
| 650          | 8.445                | 4.81%| organic silicon compound Si–X stretching vibration |
| 674          | 13.490               | 7.69%| C–H bending vibration of benzene |
| 698          | 16.787               | 9.56%| C–H bending vibration of monosubstituted benzene |
| 721          | 26.202               | 14.93%| C–H bending vibration of m-disubstituted benzene |
| 743          | 24.909               | 14.19%| C–H bending vibration of m-disubstituted benzene |
| 765          | 26.780               | 15.26%| aromatic heterocyclic ring stretching vibration |
| 789          | 24.372               | 13.89%| C–H bending vibration of m-disubstituted benzene |
| 814          | 10.940               | 6.23%| aromatic heterocyclic ring stretching vibration |
| 841          | 10.211               | 5.82%| C–H bending vibration of p-disubstituted benzene |
| 871          | 13.387               | 7.63%| C–H bending vibration of pentasubstituted benzene |
| sample point 12 |                   |      |               |
| 649          | 9.255                | 5.64%| organic silicon compound Si–X stretching vibration |
| 676          | 16.043               | 9.78%| C–H bending vibration of benzene |
| 704          | 20.312               | 12.39%| C–H bending vibration of monosubstituted benzene |
| 729          | 26.777               | 16.33%| aromatic heterocyclic ring stretching vibration |
| 756          | 27.349               | 16.68%| C–H bending vibration of monosubstituted benzene |
| 782          | 23.573               | 15.60%| C–H bending vibration of m-disubstituted benzene |
| 805          | 14.765               | 9.00%| aromatic heterocyclic ring stretching vibration |
tiny molecular benzene rings, aliphatic chain hydrocarbons, aromatic hydrocarbons, tar, and other harmful pollutants. This complicates the composition of the resulting gas.35–37

From the area percentage of the sampling points 1–6 (Figure 12) obtained from the peak fitting diagram (Figure 11) and the functional group attribution table (Table 3), the Si–X bond of silicone compounds at sampling points 3 and 4 is smaller than that at the other four sampling points. This is because the sampling point is close to the wall of the simulated coal seam, and the temperature of the oxidation zone during the gasification process can reach more than 1000 °C. Under high temperatures, the silica in the simulated rock will react to break the Si–X bond.

Benzene compounds have high water solubility and are the typical organic pollutants produced during UCG. It can be seen from Figure 12 that the benzene compounds at sampling point 3 accounted for the largest proportion. This may be because sampling point No. 3 is close to the oxidation zone during the underground gasification process of the simulated coal seam. The high temperature will cause many cracks in the simulated rock layer.38 Under the action of high temperature, the vapor of benzene compounds will migrate and diffuse along these cracks so that the proportion of benzene compounds in sampling point 3 is the highest. Sampling point No. 4 has the least percentage of benzene compounds. This is because the supply direction of the gasification agent is from south to north. Under the action of airflow, the high-temperature gas will carry these pollutants to migrate and enrich in the simulated strata. Therefore, sampling point No. 4 has less benzene than No. 5 and No. 6.

According to previous studies, aromatic heterocyclic compounds can also pollute groundwater. From Figure 12, it can be seen that the area percentage of the No. 4 sampling point is 35.29% and that it shows a downward trend. This is because the simulated rock layer has a certain degree of adsorption, resulting in the reduction of the pollutant content.

3.2.2.2. Sampling Points 1–6, 1000–1800 cm⁻¹ Sub-Peak. Phenolic pollutants are typical pollutants produced upon underground gasification a high water solubility and migration tendency. Phenolic substances are produced in the process of UCG mainly from three aspects.39–41 First, the coal used for gasification contains certain phenolic hydroxyl substances; Second, the gasification temperature is lower than that required for ether bond breaking (C–O–C), forming high-energy and unstable molecular fragments. These molecules will release their energy from relatively stable rings of phenol, alkyl phenol, and other phenols. When the gasification temperature was over 450 °C cracking happens and by alkyl phenol and secondary hydroxyl reactions, low-grade phenols with simple structure and small molecular weight were produced; Third, in the process of UCG, the temperature in the central zone of gasification can reach more than 1000 °C, and temperatures higher than that will make PAHs crack. Its products will react with oxygen-containing functional groups to produce phenolic substances.

According to the area percentage diagram (Figure 14) of sampling points 1–6 obtained from the peak fitting diagram (Figure 13) and the functional group attribution table (Table 4), the proportion of phenolic pollutants at sampling point 3 is the largest and shows a decreasing trend to the south. Moreover, no phenolic pollutants were detected at sampling point 1. This indicates that the phenolic pollutants migrate and diffuse to the simulated rock layer around the simulated coal seam. The maximum vertical distance of migration and diffusion from the gasification reaction area to the south is about 0.7 m. Campbell’s research found that aromatic hydrocarbons are also organic pollutants produced by UCG. It can be seen from Figure 14 that the maximum percentage of aromatic pollutants at sampling point 3 is 40.27%. After that, it shows a downward trend along with the simulated rock formation to the south and shows a trend of the first decline and then increase toward the north. Compared with phenolic pollutants, the migration and diffusion distance of aromatic pollutants is higher than that of phenolic pollutants, which indicates that the simulated rock layer has a strong adsorption for phenolic pollutants, leading to a smaller migration distance. This is consistent with the results of XRD.

3.2.2.3. Sampling Points 7–12, 600–900 cm⁻¹ Sub-Peak. From the area percentage diagram of sampling points 7–12 (Figure 16) obtained from the peak fitting diagram (Figure 15) and the functional group attribution table (Table 5), the change in Si–X bond at sampling points 7–9 and 10–12 is consistent with that at sampling points 1–6. In contrast, the change in benzene and aromatic heterocyclic compounds is different. Sampling points 7 and 10 are located on both sides of the simulated coal seam, 10 cm away from the coal wall, and are in the central area of the gasification reaction. Under heat, the cracks developed in the simulated rock layer provide channels for the migration of the gaseous pollutants. During the gasification process, if the gasification agent is injected at a pressure not less than the hydrostatic pressure of the coal seam, the gas generated by the gasification process will penetrate the surrounding formation media through these fissures and cause pollution. From the percentage of area shown in Figure 16, it can be seen that the benzene and aromatic heterocyclic compounds show opposite trends. This shows that benzene pollutants migrate and enrich easily than aromatic heterocyclic compounds.

(4) Sampling points 7–12, 1000–1800 cm⁻¹ sub-peak. The gas produced by UCG contains a lot of macromolecular organic matter produced by coal pyrolysis. The more the volatile products are produced, the farther they penetrate the surrounding rock layers before dissolving into groundwater. There are three main sources for the formation of PAHs during the UCG process.42–44 First, the raw coal itself contains a small amount of PAHs. Under the gasification conditions, inevitably there will be some PAHs that do not react and are discharged with coal gas and seimore. Second, under high temperatures, the olefin and alkyn generated by coal decomposition continue to decompose into free radical groups. These free radical groups will form low-grade aromatic rings after dehydrogenation and recombination, which will further polymerize to generate PAHs. Third, coal molecules are a network structure, which will be decomposed into small molecules without rings and with a ring under gasification conditions. After the cyclization reaction, the small molecules without rings can also produce PAHs.

From the area percentage diagram of sampling points 7–12 obtained from the peak fitting diagram (Figures 17 and 18) and
the functional group attribution table (Table 6), it can be seen that the change in aromatic hydrocarbon pollutants first decreases and then increases from the gasification center area to the east, while it is just the opposite to the west. The area percentage of phenols and aldehydes from the gasification reaction center to the east and west sides shows an increasing trend. The area percentage of the two pollutants is roughly the same. This shows that the phenol and aldehyde migration and enrichment degree is roughly the same on the east and west sides.

4. PREVENTION AND CONTROL OF POLLUTANTS

The generation, migration, and enrichment of UCG pollutants mainly depend on the fracture development pattern of the surrounding rock under the thermal action during gasification, the adsorption characteristics of the surrounding rock, the extension of the gasification working surface, the gas injection pressure, and the elemental composition of the coal. Therefore, in the actual production stage, the detailed study of the elemental composition of gasified coal, the scientific site selection of the gasified coalfield, and the selection of gasification technology are very important to prevent pollution by UCG.

The following measures can be taken to prevent and control this problem: (1) Scientific site selection before gasification. Before gasification, the condition of the gasification coal seam should be fully evaluated and there should be a certain thickness of dense water-proof layer between it and the underground aquifer. The gasification area should not contain important aquifers (poor water quality, less water volume, and environmentally and economically important aquifers) and the groundwater area of the gasification area should be at a low point than the regional groundwater level. (2) Scientific process control during gasification. In the process of gasification, gaseous pollutants mainly migrate and escape along with the gas and hence the gasification pressure should be controlled to be less than or equal to the hydrostatic pressure of the coal seam to seal the pollutants in the gasification reaction zone to reduce the diffusion of pollutants. (3) Pollutant treatment after gasification.
After gasification, the generation of pollutants can be reduced by accelerating the cooling of the combustion cavity to suppress pressure rise. Pumping polluted water from the combustion area and the surrounding strata to the ground for treatment effectively removes highly mobile pollutants.45–47

5. CONCLUSIONS

According to the analysis and detection of coal seam surrounding rock under the gasification simulation experiment of No. 7 coal in Tianjin Qianjiaying Mine, the following conclusions can be drawn:

(1) After underground gasification and the high-temperature reaction of Qianjiaying No. 7 coal seam, benzene, phenols, aldehydes, aromatic hydrocarbons, and aromatic heterocyclic compounds were found through the detection of the surrounding rock around the coal seam, of which aromatic pollutants are the main pollutants.

(2) On the east and west sides of the gasification center, the migration and enrichment of phenols and aldehydes are roughly the same. At the same time, benzene pollutants are easier to migrate and enrich than aromatic heterocyclic compounds, which indicates that the prevention and control of benzene pollutants should be

| sample point | center (cm⁻¹) | area | area | structure |
|--------------|--------------|------|------|-----------|
| sample point 7 | 1036         | 6.241 | 4.13% | C–O–C bond stretching vibration of ethers |
|               | 1140         | 34.830 | 23.04% | C–O–C bond stretching vibration of ethers |
|               | 1350         | 6.473 | 4.28% | O–H bond bending vibration of phenols |
|               | 1418         | 33.388 | 22.09% | C–H bond bending vibration of olefins |
|               | 1469         | 32.141 | 21.26% | bending vibration of methyl C–H bond |
|               | 1535         | 14.837 | 9.82% | aromatic hydrocarbon benzene ring skeleton vibration |
|               | 1622         | 15.922 | 10.53% | aromatic hydrocarbon benzene ring skeleton vibration |
|               | 1696         | 7.323 | 4.84% | C=O bond stretching vibration of aldehydes |
| sample point 8 | 1027         | 25.089 | 17.74% | C–O–C bond stretching vibration of ethers |
|               | 1138         | 35.816 | 25.33% | C–O–C bond stretching vibration of ethers |
|               | 1375         | 3.557 | 2.52% | O–H bond bending vibration of phenols |
|               | 1434         | 42.766 | 30.25% | bending vibration of methyl C–H bond |
|               | 1503         | 20.029 | 14.17% | aromatic hydrocarbon benzene ring skeleton vibration |
|               | 1625         | 11.837 | 8.37% | aromatic hydrocarbon benzene ring skeleton vibration |
|               | 1691         | 2.280 | 1.63% | C=O bond stretching vibration of aldehydes |
| sample point 9 | 1017         | 72.855 | 26.27% | C–O–C bond stretching vibration of ethers |
|               | 1135         | 71.977 | 25.95% | C–O–C bond stretching vibration of ethers |
|               | 1243         | 20.655 | 7.44% | aromatic hydrocarbon benzene ring skeleton vibration |
|               | 1332         | 16.397 | 5.91% | O–H bond bending vibration of phenols |
|               | 1437         | 45.290 | 16.33% | bending vibration of methyl C–H bond |
|               | 1528         | 16.645 | 6.00% | aromatic hydrocarbon benzene ring skeleton vibration |
|               | 1639         | 20.632 | 7.44% | aromatic hydrocarbon benzene ring skeleton vibration |
|               | 1761         | 12.898 | 4.65% | C=O bond stretching vibration of aldehydes |
| sample point 10 | 1026        | 32.803 | 16.25% | C–O–C bond stretching vibration of ethers |
|                | 1138        | 64.487 | 31.94% | C–O–C bond stretching vibration of ethers |
|                | 1406        | 24.129 | 11.95% | bending vibration of alkane C–H Bond |
|                | 1449        | 41.464 | 20.54% | bending vibration of methyl C–H bond |
|                | 1512        | 18.661 | 9.24% | aromatic hydrocarbon benzene ring skeleton vibration |
|                | 1625        | 16.227 | 8.04% | aromatic hydrocarbon benzene ring skeleton vibration |
|                | 1696        | 4.127 | 2.04% | C=O bond stretching vibration of aldehydes |
| sample point 11 | 1030        | 60.900 | 19.16% | C–O–C bond stretching vibration of ethers |
|                | 1116        | 49.055 | 15.43% | C–O–C bond stretching vibration of ethers |
|                | 1164        | 44.228 | 13.91% | C–O–C bond stretching vibration of ethers |
|                | 1376        | 9.849 | 3.10% | O–H bond bending vibration of phenols |
|                | 1426        | 55.766 | 17.54% | bending vibration of methyl C–H bond |
|                | 1475        | 48.729 | 15.33% | bending vibration of C–H bond of methine |
|                | 1532        | 20.786 | 6.54% | aromatic hydrocarbon benzene ring skeleton vibration |
|                | 1621        | 19.838 | 6.24% | aromatic hydrocarbon benzene ring skeleton vibration |
|                | 1684        | 8.771 | 2.76% | C=O bond stretching vibration of aldehydes |
| sample point 12 | 1035        | 13.863 | 5.17% | C–O–C bond stretching vibration of ethers |
|                | 1141        | 54.710 | 20.40% | C–O–C bond stretching vibration of ethers |
|                | 1349        | 12.218 | 4.55% | O–H bond bending vibration of phenols |
|                | 1425        | 63.164 | 23.55% | bending vibration of methyl C–H bond |
|                | 1479        | 48.743 | 18.17% | bending vibration of C–H bond of methane |
|                | 1544        | 25.671 | 9.57% | aromatic hydrocarbon benzene ring skeleton vibration |
|                | 1626        | 34.322 | 12.80% | aromatic hydrocarbon benzene ring skeleton vibration |
|                | 1700        | 15.550 | 5.80% | C=O bond stretching vibration of aldehydes |

Table 6. The Functional Group Attribution of 1000–1800 cm⁻¹ at Sampling Points 7–12
strengthened during actual gasification production to reduce their pollution around the fuel–air area.

(3) In the south of the gasification area, the migration distance of phenolic pollutants is less than that of other pollutants. The maximum vertical distance of its migration and diffusion from the gasification reaction area to the south is about 0.7 m.

(4) Before proceeding to UCG, a detailed study of the elemental composition of the gasified coal, scientific selection of the gasification coalfield, and scientific selection of the gasification process are very important links in preventing pollution by UCG.

■ AUTHOR INFORMATION

Corresponding Author

Lin Xin – College of Safety and Environmental Engineering and Key Laboratory of Ministry of Education for Mine Disaster Prevention and Control, Shandong University of Science and Technology, Qingdao, Shandong 266590, China; Email: xinlinsdust@sdu.edu.cn

Authors

Kaixuan Li – College of Safety and Environmental Engineering, Shandong University of Science and Technology, Qingdao, Shandong 266590, China

Mingze Feng – College of Safety and Environmental Engineering, Shandong University of Science and Technology, Qingdao, Shandong 266590, China

Weimin Cheng – College of Safety and Environmental Engineering and Key Laboratory of Ministry of Education for Mine Disaster Prevention and Control, Shandong University of Science and Technology, Qingdao, Shandong 266590, China

Zhigang Wang – North China Geological Exploration Bureau of Tianjin, Tianjin 300170, China

Jiaze Li – College of Safety and Environmental Engineering, Shandong University of Science and Technology, Qingdao, Shandong 266590, China

Jing Wu – College of Safety and Environmental Engineering, Shandong University of Science and Technology, Qingdao, Shandong 266590, China

Complete contact information is available at: https://pubs.acs.org/10.1021/acsomega.2c01135

Notes
The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

This study was financially supported by the Shandong Natural Science Foundation (No. ZR2020ME084), the National Natural Science Foundation of China (No. 51504142), the Qinghuang Science and Technology Program of Shandong Province University (No. 2019KJG008), the SDUST Research Fund (No. 2018TDJ1H102), and the Geological Survey Project of China Geological Survey (No. DD20190182).

■ REFERENCES

(1) Han, S.; Chen, H.; Long, R.; Cui, X. Peak coal in China: A literature review. Resour. Conserv. Recycl. 2018, 129, 293–306.

(2) Wang, J.; Dong, X.; Dong, K. How renewable energy reduces CO2 emissions? Decoupling and decomposition analysis for 25 countries along the Belt and Road. Appl. Econ. 2021, 53, 4597–4613.

(3) Heede, R.; Oreskes, N. Potential emissions of CO2 and methane from proved reserves of fossil fuels: An alternative analysis. NATO ASI Ser., Ser. I 2016, 36, 12–20.

(4) Liu, H.; Liu, S. Life cycle energy consumption and GHG emissions of hydrogen production from underground coal gasification in comparison with surface coal gasification. Int. J. Hydrogen Energy 2021, 46, 9630–9643.

(5) Krause, E.; Krzemień, A.; Smoliński, A. Analysis and assessment of a critical event during an underground coal gasification experiment. J. Loss Prev. Process Ind. 2015, 33, 173–182.

(6) Bazaluk, O.; Lozynskyi, V.; Falshhtynskyi, V.; Saik, P.; Dychkovskyi, R.; Cabana, E. Experimental studies of the effect of design and technological solutions on the intensification of an underground coal gasification process. Energies 2021, 14, 4369.

(7) Jiang, L.; Chen, Z.; Ali, S. M. F. Feasibility of carbon dioxide storage in post-burn underground coal gasification cavities. Appl. Energy 2019, 252, No. 113479.

(8) Falshhtynskyi, V.; Saik, P.; Lozynskyi, V.; Dychkovskyi, R.; Petlovanyi, M. Innovative aspects of underground coal gasification technology in mine conditions. Mining of Mineral Deposits 2018, 12, 68–75.

(9) Huang, W.; Wang, Z.; Xie, T.; Du, X. Feasibility study on underground coal gasification of quality characteristics of 9 Chinese coal types. Energy Sources, Part A 2020, 42, 131–152.

(10) ŠkavecKová, E.; ToMašKOVá, M.; Wittenberger, G.; Zelenák, Š. Analysis of risk factors for underground coal gasification. Management Systems in Production Engineering 2019, 27, 227–235.

(11) Zou, C.; Chen, Y.; Kong, L.; Sun, F.; Chen, S.; Dong, Z. Underground coal gasification and its strategic significance to the development of natural gas industry in China. Pet. Explor. Dev. 2019, 46, 205–215.

(12) Xin, L.; Li, J.; Xie, J.; Li, C.; Han, L.; An, M.; Xu, M.; Wang, Z. Simulation of cavity extension formation in the early ignition stage based on a coal block gasification experiment. ASME: J. Energy Resour. Technol. 2020, 142, No. 062304.

(13) Strugala-Wilczek, A.; Stanczyk, K. Comparison of metal elution from cavern residue after underground coal gasification and from ash obtained during coal combustion. Fuel 2015, 158, 733–743.

(14) Li, J.-G.; Gao, B.-P.; Wang, Y.-Y.; Wei, H.-R.; Zhao, J. Experimental research on pollutants precipitation of underground coal gasification. J. China Coal Soc. 2012, 37, 173–177.

(15) Kapusta, K.; Stańczyk, K.; Wiątowski, M.; Chečko, J. Environmental aspects of a field-scale underground coal gasification trial in a shallow coal seam at the Experimental Mine Barbara in Poland. Fuel 2013, 113, 196–208.

(16) Űtnö, Y. E.; Okutan, H.; Aydın, A. A. Polycyclic aromatic hydrocarbon (PAH) content of Malkara lignite and its ex-situ underground coal gasification (UCG) char residues. Fuel 2020, 275, No. 117949.

(17) Ma, W.; Liu, S.; Li, Z.; Lv, J.; Yang, L. Release and transformation mechanisms of hazardous trace elements in the ash and slag during underground coal gasification. Fuel 2020, 281, No. 118774.

(18) Liu, S.; Niu, M.; Qi, K.; Song, X.; Li, J.; He, Y.; Wang, Z.; Gao, B. Migration behavior of typical pollutants from underground coal gasification. J. China Coal Soc. 2018, 43, 2618–2624.

(19) Ye, Y.; Chen, L.; Xing, B.; Yi, G.; Xu, B.; Li, Z.; Zhang, L. Research on the pollution from underground bituminous coal gasification. Applied Chemical Industry 2016, 45, 1424–1427+1430.

(20) Liu, S.; Ma, W. Leaching characteristics of hazardous trace elements in the slag from oxygen-enriched underground coal gasification. J. China Coal Soc. 2020, 45, 4201–4208.

(21) Li, Z.-X.; Chen, L.-J.; Ye, Y.-N.; Xu, B.; Liu, K.; Zhang, L.; Liu, J.-W.; Su, Y. Dissolution of pollutants from large semi-coke particles in groundwater. Chem. Eng. 2016, 44, 58–63.

(22) Sadasivam, S.; Zagorčak, R.; Thomas, H. R.; Kapusta, K.; Stańczyk, K. Characterisation of the Contaminants Generated from a Large-Scale Ex-Situ Underground Coal Gasification Study Using High-Resolut-Coal from the South Wales Coalfield Water, Air, & Soil Pollution: An International. J. Environ. Pollut. 2020, 231, 43–51.
(23) Chen, L.; Li, C.; Xu, B.; Xing, B.; Yi, G.; Huang, G.; Zhang, C.; Liu, J. Microbial degradation of organic pollutants in groundwater related to underground coal gasification. *Energy Sci. Eng.* 2019, 7, 2098–2111.

(24) Hou, G.; Liang, J.; Jing, H.; Tan, J.; Zhang, Y.; Yang, X.; Xie, X. Influence of Deviatoric Stress on the Deformation and Damage Evolution of Surrounding Rock under Unloading Conditions. *Shock and Vibration* 2020, 2020, 1–14.

(25) An, W.; Wang, L.; Liu, X.; Pan, J.; Li, X. Analysis the Structural Characteristics of Fuxin Long Flane Coal Based on FTIR and XRD Experiments. *Polym. Bull.* 2018, 3, 67–74.

(26) Li, Q.; Lin, B.; Zhao, C.; Wu, W. Chemical Structure Analysis of Coal Char Surface Based on Fourier-Transform Infrared Spectrometer. *Proc. CSEE* 2011, 31, 46–52.

(27) Imran, M.; Kumar, D.; Kumar, N.; Quyyum, A.; Saeed, A.; Bhatti, M. S. Environmental concerns of underground coal gasification. *Renewable Sustainable Energy Rev.* 2014, 31, 600–610.

(28) Xu, B.; Chen, L.; Xing, B.; Li, L.; Zhang, L.; Wang, X.; Chen, H.; Yi, G.; Huang, G. The environmental effect of underground coal gasification semi coke on confined groundwater. *Environ. Prog. Sustainable Energy* 2016, 35, 1584–1589.

(29) Mellors, R.; Yang, X.; White, J. A.; Ramirez, A.; Wagoner, J.; Camp, D. W. Advanced geophysical underground coal gasification monitoring. *Mitig. Adapt. Strateg. Glob. Change* 2016, 21, 487–500.

(30) Xu, M.; Xin, L.; Liu, W.; Hu, X.; Cheng, W.; Li, C.; Wang, Z. Study on the physical properties of coal pyrolysis in underground coal gasification channel. *Powder Technol.* 2020, 376, 573–592.

(31) Agarwal, M.; Kudapa, V. K.; Sudharsan, J. Analytical study of structural characteristics of South Eastern coal field by FTIR spectroscopy and X-ray diffraction. *Mater. Today: Proc.* 2021, 47, 5319–5325.

(32) Zhang, Y.; Wang, J.; Xue, S.; Wu, J.; Chang, L.; Li, Z. Kinetic study on changes in methyl and methylene groups during low-temperature oxidation of coal via in-situ FTIR. *Int. J. Coal Geol.* 2016, 154, 155–164.

(33) Akbarzadeh, H.; Chalaturnyk, R. J. Structural changes in coal at elevated temperature pertinent to underground coal gasification: A review. *Int. J. Coal Geol.* 2014, 131, 126–146.

(34) Smolińska, A.; Stańczyk, K.; Kapusta, K.; Howaniec, N. Chemometric Study of the Ex Situ Underground Coal Gasification Wastewater Experimental Data. *Water, Air, Soil Pollut.* 2012, 223, 5745–5758.

(35) Pankiewicz-Sperka, M.; Stańczyk, K.; Plaza, G. A.; Kwasniowska, J.; Nalcz-Jawecki, G. Assessment of the chemical, microbiological and toxicological aspects of post-processing water from underground coal gasification. *Ecotoxicol. Environ. Saf.* 2014, 108, 294–301.

(36) Ma, W.; Li, Z.; Lv, J.; Yang, L.; Liu, S. Environmental evaluation study of toxic elements (F, Zn, Be, Ni, Ba, U) in the underground coal gasification (UCG) residuals. *J. Cleaner Prod.* 2021, 297, No. 126565.

(37) Durdán, M.; Laciak, M.; Kačur, J.; Flegner, P.; Kostúr, K. Evaluation of synthetic gas harmful effects created at the underground coal gasification process realized in laboratory conditions. *Measurement* 2019, 147, No. 106866.

(38) Xin, L.; Li, C.; Liu, W.; Xu, M.; Xie, J.; Han, L.; An, M. Change of sandstone microstructure and mineral transformation nearby UCG channel. *Fuel Process. Technol.* 2021, 211, No. 106575.

(39) Zheng, M.; Li, X.; Guo, L. Dynamic trends for char/soot formation during secondary reactions of coal pyrolysis by large-scale reactive molecular dynamics. *J. Anal. Appl. Pyrolysis* 2021, 155, No. 105048.

(40) Wang, G.; Zhou, A. Time evolution of coal structure during low temperature air oxidation. *Int. J. Min. Sci. Technol.* 2012, 22, S17–S21.

(41) Richter, H.; Howard, J. B. Formation of polycyclic aromatic hydrocarbons and their growth to soot—a review of chemical reaction pathways. *Prog. Energy Combust. Sci.* 2000, 26, 565–608.

(42) Sun, J.; Feng, H.; Xu, J.; Jin, H.; Guo, L. Investigation of the conversion mechanism for hydrogen production by coal gasification in supercritical water. *Int. J. Hydrogen Energy* 2021, 46, 10205–10215.