Structural Evolution of Hydrocarbon-Rich Coal of the Late Carboniferous Taiyuan Formation in Dongpu Sag

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ABSTRACT: The coal system of the Taiyuan Formation in the Dongpu Sag is a good source rock. In this paper, the representative hydrogen-rich coal of the Taiyuan Formation is selected for pyrolysis experiments. We used high-resolution transmission electron microscopy and Fourier transform infrared spectroscopy to characterize the structural evolution of coal during thermal simulation, combined with the characteristics of gas and liquid products from low-maturity coal pyrolysis to comprehensively reveal the process of coal of the Taiyuan Formation to hydrocarbon. The results show that the evolution of a hydrogen-rich coal structure is mainly divided into five stages: (1) Before 350 °C: The content of aromatic hydrogen and the distance between aromatic layers are almost unchanged. The aromatic structure is mainly composed of naphthalene and $2 \times 2$ aromatic rings, indicating that polycondensation does not clearly occur. Liquid hydrocarbons reach their maximum amount due to liptinite cracking. (2) 350−400 °C: The aromatic layer distance rapidly decreases, indicating that considerable polycondensation occurs. The fatty acid hydrogen in vitrinite is gradually reduced, which is caused by cracking of the side chain of the vitrinite fat to generate gaseous hydrocarbons. The rapid decline in liquid hydrocarbons and total hydrocarbons and the rapid increase in the aromatic hydrogen content of vitrinite may be caused by the cyclization and aromatization of the long-chain fatty acid structure, which converts the liquid hydrocarbons back to a solid. (3) 400−450 °C: The aromatic layer distance is almost unchanged. The fatty acid hydrogen in vitrinite slowly decreases, and the aromatic hydrogen in vitrinite gradually increases. The large amount of gaseous hydrocarbon generated at this stage is partly due to the continued cleavage of the fatty acid side chains in vitrinite and partly from the cleavage of the fatty acid side chains from the solid formed by aromatization. (4) 450−550 °C: The aromatic layer distance rapidly decreases to the minimum, and aromatic rings with sizes above $4 \times 4$ increase rapidly. Aromatic hydrogen rapidly decreases to the minimum, and the fatty acid hydrogen of vitrinite quickly decreases to 0. Considerable polycondensation and demethylation reactions occur in the vitrinite to produce a large amount of gaseous hydrocarbon. (5) 550−600 °C: The aromatic layer distance and contents of fatty acid hydrogen and aromatic hydrogen in vitrinite change slowly. Additionally, the yields of gas and liquid do not change significantly, indicating that the polycondensation intensity decreases and that the vitrinite and liptinite are cracked without producing hydrocarbons.

1. INTRODUCTION

Coal has strong heterogeneity. Coals in different regions have different structural types, and coals with different maturities in the same region also have different structural types. The complex and heterogeneous nature of coal makes its structural characterization very challenging.1−3 Coal chemists believe that hydrogen-rich coal is equivalent to type II kerogen, and petroleum geologists believe that coal is equivalent to type III kerogen. Previous discussions on the hydrocarbon generation
potential of hydrogen-rich coal still show many disagreements, but in the final analysis, the hydrocarbon generation potential of coal depends on the structural characteristics of coal. In view of the above problems, this study mainly selected the structural evolution of hydrocarbon-rich coal of the Late Carboniferous Taiyuan Formation.

Macerals can behave differently upon heating. In general, the aliphatic fraction is gradually removed, while the aromatic materials coalesce into large clusters during the coalsification process. Fourier transform infrared (FTIR) spectroscopy provides important information on molecular structure, especially the functionalities of organic compounds and the liquid products of coal processing. Functional groups resulting from the oxidation of coal are detected using various analytical techniques, mainly FTIR spectroscopy. HRTEM spectroscopy was used to study the structural parameters of nine coal samples from a contact metamorphic zone. The aromatic structure of coal increases and the aliphatic structure decreases during metamorphic evolution. As the coal samples increase in rank, KBr-FTIR spectra exhibit an increase in aromaticity and an enhanced condensation of aromatic rings, whereas the aliphatic chain length and the “C” factor decrease.

Before being applied to the structural characterization of coal, high-resolution transmission electron microscopy (HRTEM) was used to study the microstructure of kerogen, coke, and graphite. HRTEM has been used to evaluate the molecular structure and molecular weight distribution of specific coal samples. The molecular weight distribution of Pocahontas No. 3 low-volatile bituminous coal was obtained through the use of HRTEM and laser desorption ionization mass spectrometry. HRTEM can successfully quantify the structural change in coal after heat treatment. The structural transformations in three coal components, barkinite, vitrinite, and resinite, after heat treatment from 200 to 700 °C have been investigated through the use of HRTEM. Most of the work discussed has been based on image analysis of lattice fringe micrographs that are extracted from the original micrograph by image processing techniques.

After nearly 40 years of exploration, a large number of coal-formed gas reservoirs have been discovered in Dongpu Sag. Although the predecessors have made a lot of scientific achievements in identifying the hydrocarbon generation and expulsion characteristics of coal-derived gas, there are still many problems to be solved urgently for the structural evolution of coal-based source rocks and the mechanism of hydrocarbon generation: (1) To study the structural evolution characteristics of the solid residue of coal during pyrolysis and (2) to explore the relationship between the structural evolution of hydrogen-rich coal and gas–liquid products.

2. RESULTS AND DISCUSSION

2.1. Gas–Liquid Hydrocarbon Yield in the Pyrolysis Experiment. Table 1 shows the hydrocarbon generation yield of hydrogen-rich coal in the thermal model experiment. The yield change in total hydrocarbons is mainly divided into two sections. The temperature at 400 °C is the dividing line. The change curve of total hydrocarbons before 400 °C is consistent with that of liquid hydrocarbons. The change curve of total hydrocarbons after 400 °C is consistent with gaseous hydrocarbons (Figure 1). Before 300 °C, the yield of liquid hydrocarbons increases rapidly to 167.48 mg/g TOC and the yield of gaseous hydrocarbons is very low. At this stage, liptinite cracked to produce oil. From 300 to 400 °C, the yield of liquid hydrocarbons decreases rapidly from 167.48 to 42.87 mg/g TOC and the yield of gaseous hydrocarbons slowly increases to 56.49 mg/g TOC at 400 °C. At this stage, the decrease in liquid hydrocarbons is due to partial cracking to generate gaseous hydrocarbons while the fatty acid chains in some of the liquid hydrocarbons are aromatized back to solids. The above combination of factors decreases the total hydrocarbon yield.

From 400 to 450 °C, the yield of gaseous hydrocarbons increases rapidly and reaches 140.57 mg/g TOC at 450 °C. The liquid hydrocarbons slowly change, indicating that the production of gaseous hydrocarbons has little correlation with that of liquid hydrocarbons. From 450 to 550 °C, the amount of liquid hydrocarbons slowly decreases. The yield of liquid hydrocarbons is almost 0 at 500 °C, and the yield of gaseous hydrocarbons slowly increases to 179.76 mg/g TOC at 550 °C. From 550 to 600 °C, the changes in the amount of gaseous hydrocarbons and liquid hydrocarbons are relatively slow and the hydrocarbon generation potential is almost exhausted.

2.2. Microscopic Characteristics of the Coal Samples. SD-1 has strong fluorescence (Figure 2a), and liptinite is identified mainly as algae and sporophytes under a microscope. The microscopic components of SD-1 have complete shapes and strong fluorescence, indicating that it has a strong hydrocarbon generation potential. The fluorescence intensity of SD-1 at 250 °C decreases significantly (Figure 2b), indicating liptinite begins to generate hydrocarbons at 250 °C. Most of the liptinite is reddish-brown and has large pores on the surface. A few algae residues still show fluorescence. Crustaceans are cracked to produce liquid hydrocarbons before...
300 °C. From 300 to 350 °C, under a microscope, the fluorescence of liptinite is weak.

The morphology of the sporophytes, horny bodies, and algae is blurred (Figure 2c,d). The liptinite has basically been cracked. Thus, the change in coal structure is mainly related to the hydrocarbon generation of the liptinite. From 350 to 600 °C, no fluorescence is observed under the microscope, and the pores of the vitrinite are observed to be increasingly developed (Figure 2e–h), indicating that the changes in coal structure after 350 °C are mainly related to vitrinite.

2.3. HRTEM Characterization of the Coal Samples.
2.3.1. PCAS Software Processing of the HRTEM Images.

Figure 3 shows two methods for processing HRTEM images: MAPGIS; (g) fringe-extracted image by PCAS; and (h) colored image by PCAS.

Figure 4. Diagram of aromatic parallelogram structure corresponding to different fringe lengths.

This study used PCAS fracture pore image recognition software for processing and analysis. The length and parameter

Figure 2. Microscopic characteristics of coal samples at different temperatures: (a) sporophytes and algae; (b, c) fluorescence of liptinite; (d–f) liptinite is cracked completely without fluorescence; (g) vitrinite cracking creates a lot of pores; and (h) large holes in the vitrinite group.
settings recognized by PCAS are in pixels. The actual length \((C)\) can be converted from the pixel length \((C)\) and resolution of the image \((P)\).

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C' = C/P
\]

The resolution of the image processed by HRTEM in this experiment is \(P = 37.79\) pixels/\(\mu m\). Through the above conversion, the actual value of each aromatic fringe can be obtained.

Different lengths of aromatic fringe correspond to different sizes of aromatic rings. The method proposed by Mathews et al. was used to assign aromatic sizes to the extracted HRTEM fringes. This method assumes that the aromatic fringes are in the shape of parallellograms. Note that the parallellogram-shaped aromatic sheets are not the true representation of the aromatic units in coal, but only a method that can be used as a starting point for representing the diversity and distribution of the aromatic units present in coal. Each hand-extracted fringe was assigned to an aromatic parallellogram according to its size. For example, all fringes between 3.0 and 5.4 Å were assigned to naphthalene and fringes between 5.5 and 7.4 Å were assigned to \(2 \times 2\) (Figure 4). Based on this distribution, Table 2 shows the statistics of different aromatic ring sizes for the 250 and 300 °C coal samples, as identified by PCAS and MAPGIS. Through a comparison, the results obtained by automatic PCAS identification and MAPGIS identification are not exactly the same, but both reflect the same trend. PCAS can recognize a certain amount of \(6 \times 6\)- and \(7 \times 7\)-sized aromatic rings, while MAPGIS recognizes \(7 \times 7\)-sized aromatic rings as 0. At 300 °C, PCAS recognizes \(2 \times 2\) as the main aromatic ring type and MAPGIS recognizes that naphthalene is still the main aromatic ring type. In general, PCAS can still identify a small number of large aromatic rings in low-rank coal. MAPGIS recognition is slightly lacking in the recognition of large-sized aromatic rings due to image resolution and sharpness. A comparative analysis shows that PCAS is more advantageous in identifying large aromatic rings and more objective and concise in identifying stripes.

2.3.2. HRTEM Image Analysis. Figure 5 shows the HRTEM micrographs and their corresponding fringe-extracted images. Figures 6 and 7 show the evolution curves showing the proportion of aromatic rings with temperature.

The content of naphthalene rings in the SD-1 and 250 °C coal samples has an absolute advantage, accounting for 77 and 56%, respectively. This is followed by \(2 \times 2\) and \(3 \times 3\) aromatic rings in which each accounts for approximately 10%; finally, the content of large aromatic rings such as \(5 \times 5\), \(6 \times 6\), and \(7 \times 7\) is almost zero. This shows that low-rank coals do not undergo drastic polycondensation reactions but mainly consist of small aromatic ring and chain structures. Before 400 °C, with increasing temperature, the naphthalene ring content decreases sharply to 8% at 400 °C. The content of \(2 \times 2\) and \(3 \times 3\) aromatic rings increases rapidly, while that of \(4 \times 4\) and above increases slowly. Small aromatic rings of naphthalene undergo polycondensation before 400 °C to produce \(2 \times 2\) and \(3 \times 3\) aromatic rings. From 400 to 600 °C, the content of naphthalene rings slowly decreases to 0; for \(2 \times 2\) aromatic rings, it decreases to 0; for \(3 \times 3\) aromatic rings, it fluctuates slowly within the range of 32–44%; and for \(4 \times 4\) and larger, it rapidly increases to a maximum of 58% at 600 °C. The structure is mainly composed of \(3 \times 3\), \(4 \times 4\), and \(5 \times 5\) aromatic rings at 600 °C. The naphthalene and \(2 \times 2\) aromatic rings undergo polycondensation reactions and continue to connect to \(3 \times 3\), \(4 \times 4\), and \(5 \times 5\) aromatic rings with larger molecular weights.

Figure 8 shows the images of roses in the direction of the aromatic ring of coal samples at various temperatures. The lines in different directions represent aromatic fringes in different directions, and the length of the lines represents the number of fringes in that direction. The distribution of the aromatic stripes at SD-1, 250, and 300 °C is mostly radial but mainly concentrated in the directions of 0 and 90°. Therefore, low-rank coal still has a certain orientation. From 350 to 600 °C, the direction of the aromatic fringe gradually becomes one direction. This shows that the direction of the lattice fringe tends to be directional and becomes gradually ordered as the temperature increases. The arrangement of the aromatic rings at each angle before 350 °C is orthogonal, indicating that the arrangement of the basic structural units of the aromatic rings at low temperatures is not completely disordered. This study found the law of orthogonal arrangement for the first time. In future modeling and research, attention should be paid to the arrangement and connection of basic structural elements of aromatic rings of low-maturity coal samples in three-dimensional space, which are not completely disordered and may be mostly orthogonal arrangement.

The coal nucleus is the basic unit of the chemical structure of coal. Aromatic ring polycondensation forms an aromatic ring layer (sheet), and its directionality gradually tends to be the same. Several closely aligned aromatic ring layers that are parallel to each other are called coal nuclei. Between the parallel aromatic layers that make up the coal nucleus, the vertical distance between the parallel aromatic layers that make up the coal nucleus is \(d_{002}\). The change trend of the layer distance can be divided into two parts: the layer distance of hydrogen-rich coal changes slowly before 350 °C, from 400 to 450 °C, and finally from 550 to 600 °C; however, from 350 to 400 and 450 to 550 °C, the layer distance rapidly decreases (Figure 9). This also corresponds to the rapid decrease in liquid and total hydrocarbons at 350–400 °C and the subsequent rapid increase in gaseous hydrocarbons from 450 to 550 °C, as shown in Figure 2. The results show that polycondensation clearly occurs in the temperature ranges of 350–400 and 450–550 °C, resulting in a continuous decrease in layer distance. The polycondensation from 350 to 400 °C is mainly caused by the cyclization and aromatization of liquid hydrocarbons into transitional substances, and the strong polycondensation at 450–550 °C is related to the demethylation of methyl groups that break off of benzene rings.

2.4. FTIR Spectra of Coal Samples at Different Temperatures. Figure 10 shows a comparison chart of the FTIR spectra of the vitrinite of nine samples. With increasing
temperature, the peak intensity of the aliphatic C–H telescopic vibration absorption peak, in the range of 3000–2800 cm\(^{-1}\) for vitrinite, gradually decreases, while the peak intensity of the aromatic C–H out-of-plane deformation vibration peak, in the range of 700–900 cm\(^{-1}\), gradually increases. The results show that with increasing temperature, the aliphatic chain structure of vitrinite is gradually broken to generate hydrocarbons, the aromatic structure is gradually polymerized, and at 600 °C, the vitrinite is mainly composed of aromatic structures.

The peak areas of aliphatic C–H (3000–2800 cm\(^{-1}\)) and aromatic C–H (900–700 cm\(^{-1}\)) of vitrinite in the thermally simulated coal residue at different temperatures were measured. The evolution of the characteristic peak area of vitrinite (Figure 11) can be divided into three stages. Before 350 °C, the aliphatic hydrogen content gradually decreases and the aromatic hydrogen changes slowly. Combined with the observation under a microscope, it is believed that the growth of liquid hydrocarbons at this stage mainly originates from the cracking of liptinite. At 300 °C, the aliphatic side chain of vitrinite is gradually cracked to generate gaseous hydrocarbons and the aliphatic hydrogen content gradually decreases. From...
350 to 400 °C, liquid hydrocarbons decrease sharply, gaseous hydrocarbons slowly increase, total hydrocarbons decrease, and the content of aliphatic hydrogen in the vitrinite slowly decreases to generate a small amount of gaseous hydrocarbons. Some of the aliphatic structures in the liquid hydrocarbons are cracked to generate gaseous hydrocarbons, and some of the long-chain aliphatic structures are aromatized back to a solid structure, which leads to a sharp decrease in liquid hydrocarbons while aromatics in the vitrinite rapidly increases.

From 400 to 450 °C, the yield of liquid hydrocarbons slowly decreases, the yield of gaseous hydrocarbons increases rapidly, the content of aliphatic hydrogen in the vitrinite slowly decreases, and the content of aromatic hydrogen gradually increases. The gas generated in this stage is not primarily produced from the cracking of the aliphatic side chain of vitrinite; therefore, the large amount of gaseous hydrocarbon generated in this stage may be related to the cracking of the aromatic side chain on the solid formed by the aromatization during the previous stage. From 450 to 550 °C, the gas hydrocarbon yield gradually increases to the maximum value of 179.76 mg/g TOC and almost no liquid hydrocarbon is produced. The content of aliphatic hydrogen in vitrinite rapidly decreases to the minimum value of 0, and the content of aromatic hydrogen also rapidly decreases to the minimum value at 550 °C. In vitrinite and inertinite, the methyl group successively falls off of the benzene ring and demethylation takes place to generate methane. A large amount of condensation takes place at the same time as demethylation, which leads to a sharp reduction in aromatic hydrogen in the vitrinite group. From 550 to 600 °C, the change in the gas–liquid hydrocarbon yield tends to be slight, and there is almost no change in the aliphatic hydrogen and aromatic hydrogen of vitrinite. At this stage, the liptinite and vitrinite, which are almost completely cracked, do not continue to generate hydrocarbons at all.

3. CONCLUSIONS

The structural evolution of the hydrogen-rich coal at the bottom of the Late Carboniferous Taiyuan Formation in Dongpu Sag is divided into five stages: (1) Before 350 °C: The liquid hydrocarbon yield increases to 166.83 mg/g TOC at 350 °C, and the gas hydrocarbon yield gradually increases from 300 °C and reaches 27.26 mg/g TOC at 350 °C. From 300 °C, the content of aliphatic hydrogen in vitrinite decreases gradually, the content of aromatic hydrogen increases rapidly, and the aromatic side chains in vitrinite crack to generate gaseous hydrocarbons. The content of aromatic hydrogen and the distance between aromatic layers are almost unchanged. The aromatic structure is mainly composed of naphthalene and 2 × 2 aromatic rings. The percentage of naphthalene and 2 × 2 aromatic rings is greater than 80%, indicating that polycondensation is not clear. Under a microscope, the fluorescence of liptinite disappears at 350 °C and liquid hydrocarbons are mainly produced by the cracking of the aliphatic chain of liptinite. (2) 350–400 °C: The content of aliphatic hydrogen in vitrinite decreases gradually, the content of aromatic hydrogen increases rapidly, and the distance...
between aromatic layers decreases rapidly, which indicates that polycondensation largely occurs. The cyclization and aromatization of long-chain aliphatic structures in the liquid hydrocarbons lead to a decrease in the total hydrocarbon yield and a sharp increase in the aromatic hydrogen content of vitrinite. Due to aromatization, the distance between aromatic layers decreases sharply and polycondensation is evident. (3) 400–450 °C: The yield of liquid hydrocarbon decreases slowly, the yield of gaseous hydrocarbon increases rapidly, the content of aliphatic hydrogen in vitrinite decreases slowly, and the content of aromatic hydrogen increases gradually. In addition to a small amount of residual liquid hydrocarbon and vitrinite, the aliphatic side chain that is carried by the solid formed in the previous stage of cycloaromatization is cracked. At the same time, the part of the cyclization back to the solid in the previous stage continues to aromatize, which increases the aromatic hydrogen content. (4) 450–550 °C: The yield of liquid hydrocarbon is almost 0, the yield of gaseous hydrocarbon increases rapidly again, the content of aliphatic hydrogen in vitrinite decreases rapidly to 0, the aromatic hydrogen decreases rapidly to the minimum value, and the distance between aromatic layers decreases sharply to the minimum value at 550 °C. Aromatic rings with sizes above 4 × 4 increase rapidly. Thus, vitrinite demonstrates substantial polycondensation in this temperature range. Demethylation of vitrinite occurs and a large number of polycondensation reactions take place to produce a large amount of methane. (5) 550–600 °C: The yields of gas–liquid hydrocarbons do not change significantly, and the contents of aliphatic hydrogen and aromatic hydrogen as well as the distance between aromatic layers of vitrinite change slowly. The liptinite and
swamp lakes were developed in the vast tidal swamps in the tidal areas, forming humus coal in the peat swamps that were widely distributed. In the late Carboniferous Taiyuan Formation in the Dongpu Sag, a series of swamp lakes and large swamp lakes were developed in the vast tidal flat. Algae coal may even form in the middle, forming candle coal, axial coal, and humus coal, especially swamp lakes are widely developed in the lower part of the Taiyuan Formation, with residual humus coal phases. In this study, the representative hydrogen-rich coal SD-1 at the bottom of the late Carboniferous Taiyuan Formation in Dongpu Sag in the central part of North China Basin was selected as the thermal simulation and coal structure evolution research object. There are two reasons for choosing hydrogen-rich coal as the research object: (1) The coal of the Permian in North China, including the Dongpu Sag, is dominated by hydrogen-rich coal. Hydrogen-rich coal is representative. (2) Hydrogen-rich coal has greater potential for hydrocarbon generation. Hydrogen-rich coal will be more meaningful for pyrolysis. The microcomposition characteristics of SD-1 were statistically quantified (Table 3). The statistical results show that the largest feature of the microscopic composition of SD-1 is the high content of liptinite, which can reach 20%. In addition, algae have also been developed with an average content of 13%, and there is a low content of inertinite with an average content of 14%. The main microscopic component is the vitrinite group in which the vitrinite matrix is the main component. The hydrogen-rich vitrinite matrix, which has yellow fluorescence, contains a large amount of crust debris. Structural vitrinite also emits brown-yellow fluorescence, indicating that in addition to the vitrinite matrix, other vitrinites also have the characteristics of hydrogen-rich vitrinites due to a conversion to saprolite (Figure 12). Therefore, considering the microscopic composition of liptinite, inertinite, and vitrinite, SD-1 has the typical characteristics of hydrogen-rich coal.

4. SAMPLES AND METHODS

4.1. Samples. During the early deposition of the Late Carboniferous Taiyuan Formation in the Dongpu Sag, the sea advanced and a large amount of saltwater swamps developed, forming humus coal in the peat swamps that were widely swamped in the tidal flat; a series of swamp lakes and large swamp lakes were developed in the vast tidal flat. Algae coal may even form in the middle, forming candle coal, axial coal, and humus coal, especially swamp lakes are widely developed in the lower part of the Taiyuan Formation, with residual humus coal phases. In this study, the representative hydrogen-rich coal SD-1 at the bottom of the Late Carboniferous Taiyuan Formation in Dongpu Sag in the central part of North China Basin was selected as the thermal simulation and coal structure evolution research object. There are two reasons for choosing hydrogen-rich coal as the research object: (1) The coal of the Permian in North China, including the Dongpu Sag, is dominated by hydrogen-rich coal. Hydrogen-rich coal is representative. (2) Hydrogen-rich coal has greater potential for hydrocarbon generation. Hydrogen-rich coal will be more meaningful for pyrolysis. The microcomposition characteristics of SD-1 were statistically quantified (Table 3). The statistical results show that the largest feature of the microscopic composition of SD-1 is the high content of liptinite, which can reach 20%. In addition, algae have also been developed with an average content of 13%, and there is a low content of inertinite with an average content of 14%. The main microscopic component is the vitrinite group in which the vitrinite matrix is the main component. The hydrogen-rich vitrinite matrix, which has yellow fluorescence, contains a large amount of crust debris. Structural vitrinite also emits brown-yellow fluorescence, indicating that in addition to the vitrinite matrix, other vitrinites also have the characteristics of hydrogen-rich vitrinites due to a conversion to saprolite (Figure 12). Therefore, considering the microscopic composition of liptinite, inertinite, and vitrinite, SD-1 has the typical characteristics of hydrogen-rich coal.

4.2. Pyrolysis Experiments. This experiment was based on a hydrothermal simulation device under closed conditions to simulate the hydrocarbon generation process of source rocks. The pyrolysis experiment device was mainly composed of a high-temperature and high-pressure hydrocarbon generation reaction system, a hydraulic control system, a hydrocarbon removal system, an automatic control and data acquisition system, and a product separation and collection system. Specific experimental steps were as follows. First, the sample was crushed into a particle diameter of 2 mm. The pieces were uniformly mixed to minimize error in the experimental results that can be caused by an uneven sample composition. After the samples were dried in an oven at a constant temperature of 50 °C for 24 h, the amount of sample added at each temperature was 80 g. Nine temperature points were selected, namely, 250, 300, 350, 400, 450, 500, 550, and 600 °C, and the reaction time was 48 h. The gaseous and liquid hydrocarbons were collected at each temperature, and the yield was calculated. Moreover, the solid residues at each temperature were collected for further structural analysis.

4.3. HRTEM. Nine samples (SD-1, 250, 300, 350, 400, 450, 500, 550, and 600 °C) were selected for this experiment. Before the experiment, the coal sample was ground to less than 200 mesh and a small part of the powder was placed in absolute ethanol with a straw before being put into an ultrasonic shaker to form a suspension. The sample suspension was dropped on a copper microgrid, and the particles were observed with HRTEM. Five to six points were selected for the observation and analysis of each sample. Since most of the samples were laminated on a microgrid carbon film, they were superimposed on multiple layers. Whenever possible, the areas with thin edges were selected for observation. A stripe extraction and length calculation were performed on the image using PCAS software.

4.4. FTIR Spectroscopy. A block sample of coal was chosen at each temperature, and it was ground and stepwise polished with 3000, 5000, and 7000 mesh sandpapers; Al powder was used for the final polishing step. The instrument used in the experiment was a Thermo Fisher Nicolet iS50 FTIR spectrometer with a continuum microscope accessory.

Table 3. Organic Petrology and Pyrolysis Parameters of SD-1

| lithology | microcomponent content (%) | TOC (%) | Ro (%) | S1 (mg/g) | S2 (mg/g) | HI (mg/g TOC) | T_{max} (°C) |
|-----------|-----------------------------|---------|--------|-----------|-----------|---------------|-------------|
| SD-1 coal | 54                          | 14      | 20     | 13        | 54.4      | 0.50          | 5.47        |
|           | 310.77                      | 430     |

Figure 12. Microscopic fluorescence characteristics of SD-1.
The experiment was performed using a micro-Fourier infrared reflection mode. A gold plate was used as the background for measurement. The resolution was 4 cm\(^{-1}\) for 256 scans during the test and analysis. The OMNIC program was used for the spectral deconvolution, curve fitting, and determination of peak areas. The obtained spectra of different components were first subjected to a Kramers–Kronig transformation and then to an automatic baseline correction; finally, parameters such as peak area and peak height were obtained.

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Notes

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