Molecular Dynamics Simulation and Gas Generation Tracking of Pyrolysis of Bituminous Coal

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ABSTRACT: To study the generation rules of organic molecules or fragments and the generation paths of some hydrocarbon gases (C$_2$H$_2$/C$_2$H$_4$) and inorganic gases (CO$_2$/H$_2$O/H$_2$/H$_2$S) in the pyrolysis process of bituminous coal at 1000−5000 K, the ReaxFF molecular dynamics module in AMS software was used to simulate the pyrolysis behavior of the Hongqingliang model, Gaojialiang model, and Wiser model. With the increase of temperature, the system potential energy decreases, the endothermic efficiency increases first and then decreases, the fragments of C$_1$−C$_4$ increase, and the gas molecules generated increase. In the pyrolysis process, the oxygen-containing functional groups and hydrogen groups formed H$_2$O and H$_2$ with the increase of temperature. H$_2$S as an intermediate product is always maintained in dynamic equilibrium. CO$_2$ comes from the decarboxylation of the carboxyl groups. When the temperature is lower than 3000 K, C$_2$H$_4$ and C$_2$H$_2$ are mainly formed by the adjacent carbon structure in coal molecules, and C$_2$H$_4$ is formed from the ethyl side chain, the naphthenic structure, and the unstable aromatic rings. C$_2$H$_2$ is formed from naphthene structures and aromatic rings with multiple side chains. When the temperature is higher than 3000 K, C$_2$H$_4$ and C$_2$H$_2$ are mainly formed by the random combination of free radicals generated by the crushing of coal molecules. The research results are of great significance to coal pyrolysis and clean utilization of coal.

1. INTRODUCTION

Coal resources are the foundation of China’s industry. As of the end of 2020, the annual output of raw coal was 3.9 billion tons, an increase of 1.4% over the previous year. It can be seen that coal will still occupy a major position in China’s energy consumption structure for a long time. Analyzing the structure and reaction characteristics of coal from the molecular scale, revealing the microscopic physical and chemical properties of coal, has become a hot topic for scholars in recent years. Coal is a kind of complex macromolecular organic matter. Its molecular structure is affected by coal-forming plants and the degree of coalification, resulting in large differences in the molecular structure of coal at different locations. In addition, the coal-forming environment will also affect the structure of coal molecules and causes the coal to be doped with different inorganic components. All these have caused the diversity and specificity of coal molecules. Therefore, it is very necessary to conduct a molecular-scale research on coal pyrolysis to provide a corresponding theoretical basis for the utilization of coal.

Coal pyrolysis is an important step in coal conversion and an indispensable link in the clean utilization. Scholars have done a large amount of research on coal pyrolysis, and some scholars have conducted related experiments to determine the products of coal pyrolysis. Solomon et al. conducted detailed experimental research on coal pyrolysis as early as 1986 and promoted the process of coal pyrolysis research, which is of great significance. Kök et al. used the thermogravimetric method to experiment on the influence of coal particle size on pyrolysis and obtained the relationship between the particle size and the coal pyrolysis rate. Serio et al. conducted an experimental study on the volatile matter produced from coal, which played an important guiding role in the related research. Duan et al. conducted a pyrolysis experiment on coal in a CO$_2$ atmosphere and proved that the CO$_2$ atmosphere promoted the conversion of C$\rightarrow$N into HCN. Meng et al. conducted an in-depth study on the chemical structure evolution during the pyrolysis and proved that the evolution of the functional group at the surface and center was quite different at 1000 °C. Xu et al. took Shenu coal as the research object and studied the reaction behavior of the aromatic structure in char under pyrolysis at different temperatures.

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Besides, some scholars used the ReaxFF module in software such as Amsterdam Modeling Suite (AMS) and Lammmps to simulate coal pyrolysis on a molecular scale. Zheng et al.\textsuperscript{15,16} used the ReaxFF module in Lammmps to simulate the pyrolysis of a large-scale lignite model composed of 4976 atoms and found that the order of appearance of gas products is H$_2$O/CO$_2$/CO/C$_2$H$_6$/CH$_4$, and the consumption of *OH and *CH$_3$ and the formation of H$_2$O and CH$_4$ have been studied in detail. Liang et al.\textsuperscript{30} proposed and optimized by van Duin et al.,\textsuperscript{30,31} which greatly improved the efficiency of the molecular reaction dynamics simulation and realized the rapid simulation of the macro-molecular system reaction. Subsequently, ReaxFF was optimized as a module and integrated into software such as AMS and Lammmps. The simple GUI and human–computer interaction facilitated the research of scientific researchers.

ReaxFF is based on the covalent formalism\textsuperscript{32} and the bond order principle, and the bond energy, bond lengths, valence angles, and torsion angle are integrated in it.\textsuperscript{33} The ReaxFF is the boundary of quantum mechanics and classical mechanics models.\textsuperscript{34} The total potential energy of the system is shown in eq 1,\textsuperscript{31} which is composed of different partial energies

$$E_{\text{system}} = E_{\text{bond}} + E_{\text{over}} + E_{\text{under}} + E_{\text{val}} + E_{\text{pen}} + E_{\text{tors}} + E_{\text{conj}} + E_{\text{vdW}} + E_{\text{Coulomb}}$$

(1)

where $E_{\text{system}}$ is the potential energy of the system. It describes the interaction between the particles of the systems which can be divided into nonreactive and reactive potentials. $E_{\text{bond}}$ represents the bond energy. It can be calculated by the bond order between the interatomic distances, which is shown in eq 2.\textsuperscript{31}

$$E_{\text{bond}} = -D_{e}^\pi \cdot BO_{ij}^\pi \cdot \exp \left[ \frac{r_{ij}}{r_{e}} \left( 1 - \left( BO_{ij}^\pi \cdot r_{e} \right)^{5/2} \right) \right] - D_{e}^\sigma \cdot BO_{ij}^\sigma$$

(2)

$BO_{ij}^\pi$ is the bond order between a pair of atoms. If a pair of atoms are carbon–hydrogen or hydrogen–hydrogen, only one sigma bond is considered, while for carbon–carbon, the bond orders of three results are one sigma and two pi bonds.

$E_{\text{over}}$ and $E_{\text{under}}$ represents overcoordinated and undercoordinated energy, respectively, as shown in eqs 4 and 5.\textsuperscript{31}

$$E_{\text{over}} = \frac{1}{1 + \exp \left( \lambda \cdot \Delta' \right)} \Delta'$$

(4)

where $E_{\text{over}} = \sum_{j=1}^{n_{\text{bond}}} BO_{ij} - \text{Val}$, is the degree of deviation for the sum of the corrected bond orders around an atomic center.

$$E_{\text{under}} = \frac{1}{1 + \exp \left( -\lambda \cdot \Delta' \right)} \Delta'$$

(5)

where $E_{\text{under}} = \sum_{j=1}^{n_{\text{bond}}} \frac{1}{1 + \exp \left( -\lambda \cdot \Delta' \right)} \Delta' BO_{ij} \cdot \Delta'$. $val$ is the valence angle energy for valence angle $i-j-k$, where $i$, $j$, and $k$ are locations for three atoms, as shown in eq 6.\textsuperscript{31}

### 2. MODELING AND COMPUTATIONAL DETAILS

#### 2.1. Optimization of Bituminous Molecular Models.

The Wiser bituminous molecular model is recognized as a relatively comprehensive and reasonable coal molecular chemical structure model, which was proposed by Wiser in 1977. The model contains aromatic structures with 1 to 5 rings. The hydrogen mainly exists in the aliphatic structures, with less aromatic hydrogen. At the same time, it contains alcohol, phenol, thiophenol, aryl ether, ketone, carboxyl, amino, and other functional groups containing O, N, and S. The connection between aromatic rings is mainly through weak bonds such as short alkane bonds (−(CH$_2$)$_n$−), ether bonds (−O−), and thioether bonds (−S−). HQL and GJL models were established during our research work, and they contain thiophenes, ether bonds (−O−), and thioether bonds (−S−). HQL and GJL models were established during our research work, and they contain thiophenes, ether bonds (−O−), and thioether bonds (−S−). HQL and GJL models were established during our research work, and they contain thiophenes, ether bonds (−O−), and thioether bonds (−S−). HQL and GJL models were established during our research work, and they contain thiophenes, ether bonds (−O−), and thioether bonds (−S−).

Here, the Wiser model is appropriately modified to increase the proportion of oxygen-containing functional groups, focusing on the reaction direction of oxygen-containing functional groups and carbon functional groups.\textsuperscript{16,27} Molecular dynamics simulation software was used to optimize the model. The parameter settings of geometry optimization, energy optimization, and annealing optimization are shown in Table 1.\textsuperscript{32,39}

#### 2.2. AMS Molecular Dynamics Simulation.\textsuperscript{20,30,31}

The ReaxFF module in AMS software was used to simulate the reaction of the pyrolysis of the bituminous models here. ReaxFF is a kind of molecular dynamics reaction force field, which was first proposed and optimized by van Duin et al.,\textsuperscript{30,31} which greatly improved the efficiency of the molecular reaction dynamics simulation.

### Table 1. Parameter Settings of Optimization

| setting   | parameter | setting   | parameter |
|-----------|-----------|-----------|-----------|
| forcefield| COMPASS II| algorithm | quasi-Newton |
| quality   | ultra-fine| max. iterations | 5000 |
| electrostatic | atom based | van der Waals atom based |
| annealing cycle | 5 | initial temperature | 298 K |
| mid-cycle temperature | 800 K | annealing steps | 5000 |
\[ E_{\text{val}} = f_1(BO_{ij}) f_2(BO_{jk}) f_3(\Delta_i) (k_\lambda - k_\lambda \exp(-k_\lambda (\Theta_{ij} - \Theta_{ij})^2)) \]

where \( f_1(BO_{ij}) = 1 - \exp(-\lambda_{ij} BO_{ij}^4) \);

\[ f_3(\Delta_i) = \frac{2 + \exp(-\lambda_{ij} \Delta_i)}{1 + \exp(-\lambda_{ij} \Delta_i) + \exp(p_{ij} \Delta_i)} \]

\[ \times \left[ \lambda_{ij} - (\lambda_{ij} - 1) \frac{2 + \exp(\lambda_{ij} \Delta_i)}{1 + \exp(\lambda_{ij} \Delta_i) + \exp(-p_{ij} \Delta_i)} \right] \]

\( E_{\text{pen}} \) is the penalty energy. It is an additional item to stabilize the system with two double bonds sharing an atom in a valence angle, as shown in eq 7.\(^{31}\)

\[ E_{\text{pen}} = \lambda_{ij} f_5(\Delta_i) \exp(-\lambda_{ij} BO_{ij} - 2^2) \exp(-\lambda_{ij} BO_{jk} - 2^2) \]

where \( f_5(\Delta_i) = \frac{2 + \exp(-\lambda_{ij} \Delta_i)}{1 + \exp(-\lambda_{ij} \Delta_i) + \exp(\lambda_{ij} \Delta_i)} \).

\( E_{\text{tors}} \) is the torsion energy. The torsion energy smoothly translates when bonds in the torsion angle break, as shown in eq 8.\(^{31}\)

\[ E_{\text{tors}} = f_6(BO_{ij}, BO_{jk}, BO_{kl}) \sin \Theta_{ij} \sin \Theta_{jk} \sin \Theta_{ik} \frac{1}{2} V_i (1 + \cos \Theta_{ij}) \]

\[ + \frac{1}{2} V_2 \exp[p_{ij} (BO_{ij} - 1 + f_{ij} (\Delta_i, \Delta_k))^2] (1 - \cos 2 \Theta_{ij}) \]

\[ + \frac{1}{2} V_3 (1 + \cos 3 \Theta_{ij}) \]

where \( \Theta_{ij} \) is the torsion angle.

\[ f_6(BO_{ij}, BO_{jk}, BO_{kl}) = (1 - \exp(-\lambda_{ij} BO_{ij}))(1 - \exp(-\lambda_{ij} BO_{jk})) \]

\[ (1 - \exp(-\lambda_{ij} BO_{jk})) \]

\[ f_{ij} (\Delta_i, \Delta_k) = \frac{2 + \exp(-\lambda_{ij} (\Delta_i + \Delta_k))}{1 + \exp(-\lambda_{ij} (\Delta_i + \Delta_k)) + \exp(-\lambda_{ij} (\Delta_i + \Delta_k))} \]

\( E_{\text{conj}} \) is the conjugate effect of the molecular energy, as shown in eq 9.\(^{31}\)

\[ E_{\text{conj}} = f_{ij} (BO_{ij}, BO_{jk}, BO_{kl}) \theta_{ij} \theta_{jk} \theta_{ik} \left[ 1 + (\cos^2 \Theta_{ij} - 1) \cdot \sin \Theta_{ij} \sin \Theta_{jk} \sin \Theta_{ik} \right] \]

where \( f_{ij} (BO_{ij}, BO_{jk}, BO_{kl}) \).

\[ = \exp(-\lambda_{ij} BO_{ij} - 1.2^2) \exp(-\lambda_{ij} BO_{jk} - 1.2^2) \]

\[ \cdot \exp(-\lambda_{ij} BO_{kl} - 1.2^2) \]

\( E_{\text{vdW}} \) is the nonbonded van der Waals interaction, as shown in eq 10.\(^{31}\)

\[ E_{\text{vdW}} = D_{ij} \left\{ \exp \left( \alpha_i \left( 1 - f_{ij} (\Theta_{ij}) \frac{r_{ij}}{r_{ij}} \right) \right) \right\} \]

\[ - 2 \exp \left\{ 1 - \alpha_i \left( 1 - f_{ij} (\Theta_{ij}) \frac{r_{ij}}{r_{ij}} \right) \right\} \]

where \( f_{ij} (\Theta_{ij}) = \frac{1}{1 + (1/\lambda_{ij} \Theta_{ij})^{4/3}} \).

\( E_{\text{Coulomb}} \) is the Coulomb interaction between all atom pairs, as shown in eq 11.\(^{31}\)

\[ E_{\text{Coulomb}} = C \cdot \sum \frac{q_i q_j}{r_{ij}^{1/3}(1 + (1/\lambda_{ij})^{4/3})^{1/5}} \]

where \( q_i \) and \( q_j \) are atomic charges.

ReaxFF describes a relationship among the bond order, bond distance, and bond energy, which relates to the dissociation and formation of the chemical bond. Based on these characteristics, the ReaxFF reactive simulation is suitable for studying the pyrolysis and combustion of coal.\(^{34}\)

The simulation here adopts the NVT Berendsen ensemble and H/C/O/N/S/B field. This force field is often used by scholars to study the process of coal pyrolysis or coal combustion and has highly adaptability. The simulation time step is set to 0.25 ps, and the iteration steps are 2 \times 10^5 steps (set no reaction in the first 3000 steps), and the total time is 50 ns. The simulated constant temperature is set to 1000, 2000, 3000, 4000, and 5000 K, respectively.

### 3. RESULTS AND DISCUSSION

The optimized unit cell structures are established, as shown in Figure 1, and each unit cell density is 1.2 g/cm\(^3\).

#### 3.1. Potential Energy of the System

The change of the pyrolysis potential energy during pyrolysis at different temperatures is shown in Figure 2. It can be seen that the higher the temperature, the lower the potential energy of the system, indicating that coal molecules obtain energy from environmental heat during the pyrolysis process, that is, the pyrolysis.

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**Figure 1.** Optimized unit cell structures. (a) Wiser (C\(_{197}\)H\(_{167}\)N\(_{3}\)O\(_{21}\)S\(_{5}\)), (b) HQL (C\(_{140}\)H\(_{116}\)N\(_{2}\)O\(_{19}\)), and (c) GJL (C\(_{140}\)H\(_{114}\)N\(_{2}\)O\(_{19}\)S\(_{2}\)).
process is an endothermic reaction. Because the reaction time is short under the simulated conditions, the coal molecule has only once chain scission at 1000 K; at 2000 K, the pyrolysis takes place further, and the reduction in potential energy is less than that at 1000 K, is 2000 kcal/mol, indicating that the endothermic efficiency is low. The potential energy curve fluctuates less, indicating that the reaction has just started, and the new reactions are less and gentle; when temperatures reach 2000−3000 and 3000−4000 K, the potential energy of the system continually reduces. The reduction exceeds 2000 kcal/mol, the potential energy curve fluctuates gradually, indicating that the heat absorption of the system reduces about 2000 K, which has decreased before, indicating that the heat absorption of the system is the largest at this time, but the endothermic efficiency is gradually reduced, the new reaction in the system is gradually reduced, and the potential energy curve fluctuates the most, indicating that the reaction is the most violent. The results show that from the beginning to the violent pyrolysis reaction, the coal molecular system will continue to absorb energy; with the temperature increasing, the endothermic efficiency first increases and then decreases, while the potential energy of the system increases, which shows that the new reactions increase first and then decrease, and the reactions become violent with the increase in temperature. The trend of potential energy change of HQ and GJ is basically the same as that of Wiser, the difference is that the potential energy interval of HQ is −37000 to −29000 and GJ is −36000 to −29000.

3.2. Reaction Products Analysis. The Wiser unit cell origin model and the final reaction product of different temperatures in the AMS simulation are shown in Figure 3.
H₂), and the system fragmentation is significantly increasing. When at 4000 K, the number of H₂O or H₂ is most, while that of at 5000 K is reduced because when the temperature reaches 5000 K, a part of H₂O or H₂ will participate in the secondary reaction and is consumed by the system.

The HQ unit cell origin model and the final reaction product of different temperatures in the AMS simulation are shown in Figure 4. Similar to Wiser, when at 1000 K, chain scission occurs only once. Starting from 2000 K, the broken chain reaction gradually increases, a large amount of hydroxyl radicals and hydrogen radicals is produced to form H₂O and H₂, and the system fragmentation is significantly increasing. Here, when at 3000 K, the number of H₂O is most, and when at 5000 K, the number of H₂ is most. With the temperature increasing, a part of H₂O will participate in the secondary reaction and is consumed by the system.

The GJ unit cell origin model and the final reaction product of different temperatures in the AMS simulation are shown in Figure 5. Its results are quite consistent with HQ, further confirming the opinion.

3.2.1. Organic Product Analysis. We ran three independent simulations for each model and counted and averaged fragments. The change in the number of fragments generated by pyrolysis of a unit cell at different temperatures is shown in Figure 6. The lower part of the figure is a stack of three simulations, and the upper part is the average of each fragment. With the increase of temperature, the number of fragments increases, indicating that the pyrolysis of coal molecules is gradually complete and the degree of fragmentation increases. The number of pyrolysis gas and small molecular fragments (C₁−C₄) increased significantly. The number of light tar fragments (C₃−C₁₅) and heavy tar fragments (C₁₆−C₄₀) always appeared and increased after 2000 K. The change of the coke fragment (C₄₀+) is not obvious, and it existed at all temperature stages. It can be concluded that high temperature promotes the secondary reaction of macromolecular fragments, which tends to produce more small fragments and gas molecules. It is basically consistent with the molecular dynamics simulation results of coal pyrolysis by Zhan et al. and Zheng et al.

3.2.2. Inorganic Product Analysis. In addition, there are some other inorganic gases generated. The main inorganic gas molecules are H₂O, CO₂, H₂S, and H₂. The number of molecules at different temperatures is shown in Figure 7. The HQL model does not contain sulfur, so H₂S is not generated. As the temperature increases, the output of H₂O and H₂ increases significantly in all models. This is because the oxygen-containing functional groups and hydrogen groups are the first to break and fall off during the gradual increase in temperature, forming °OH and °H, and so forth, and then forming H₂O and H₂; CO₂ starts appearing at 2000 K. According to the reaction pathway tracking, CO₂ mainly comes from the decarboxylation of °COOH, as shown in Table 1. In addition, CO₂ can also be formed by hydroxyl dehydrogenation and carbon atoms after high-temperature cracking; H₂S is generated after 2000 K, and after tracing the reaction pathway, it is found that almost all sulfur-containing functional groups are broken off and H₂S is maintained as an intermediate product in dynamic equilibrium.

3.2.3. Analysis of the Reaction Path of Hydrocarbons and CO₂. To further study the molecular pyrolysis of bituminous models, the AMS software was used to track the formation and release of gases during the pyrolysis process, and the formation mechanism and chemical behavior of hydrocarbons and CO₂ were obtained. Hydrocarbon gases are mainly unsaturated hydrocarbons, C₂H₄, C₃H₆, C₄H₈, in addition to a small amount of...
C2H6, and so on. When the temperature $T \leq 3000$ K, C2H4 and C2H2 are mainly formed by the adjacent carbon structure fall from the coal molecule; when the temperature $T > 3000$ K, the coal molecular system is severely destroyed and a large number of free radicals are generated, and then, they combined a large amount of C2H4, C2H2, CO2, and other gases. CO2 is mainly formed by the decarboxylation of $-\text{COOH}$ in the Wiser model, but formed by hydroxyl dehydrogenation and carbon atoms in HQL and GJL models. The main formation paths to form C2H4, C2H2, and CO2 are shown in Table 2:

Table 2: There are three main paths for C2H4 to evolve from the corresponding functional groups:

1. The $-\text{CH2CH3}$ at the $\alpha$ position of the furan structure falls off, and the $^\text{*H}$ is removed to form a double bond to generate C2H4. The furan structure is an oxygen-containing heterocyclic ring, which has poor thermal stability, and the attached side chain is $-\text{CH2CH3}$, which makes the structure more unstable. When the temperature rises, $-\text{CH2CH3}$ is the first to fall off, and the $^\text{*H}$ is directly removed to form C2H4.

2. C85 and C86 on the cycloalkane structure fall off through ring-opening and chain scission to form a double bond to generate C2H4. The four positions of naphthene are connected to another naphthene and other structures. The four adjacent positions are occupied, which makes its thermal stability poor. The C85 and C86 that are not connected to other structures fall off as a whole, directly forming C2H4.

3. The aromatic rings connected in groups are opened and broken by heating, and C1 and C6 fall off to form C2H4. The structural stability of the group aromatic rings is relatively poor, while the aromatic ring with more side chains, such as $-\text{OH}$ and $-\text{CH3}$, has worse stability. The ring with side chains is opened and broken by heating. The C1 and C6 with $-\text{OH}$ fall off as a whole, and then, $-\text{OH}$ is replaced by $^\text{*H}$ to form C2H4.

There are three main paths for C2H2 to evolve from the corresponding functional groups:

1. Similar to the second way of C2H4, C85 and C86 in the cycloalkane structure fall off through ring-opening and chain scission and continue to remove $^\text{*H}$ to form triple bonds to generate C2H2. As the temperature rises, the hydrogen atoms in the system have an obvious tendency to form $^\text{*H}$ and H2. Therefore, the degree of unsaturation of hydrocarbon gases gradually increases, and C2H4 removes $^\text{*H}$ to form C2H3.

2. Aromatic ring connecting cycloalkane is opened and broken by heating, C90 and C60 fall off, and combined with $^\text{*H}$, forming a triple bond to generate C2H2. As the temperature rises, the aromatic ring with side chains connecting the naphthenic structure and other structures begins to break. The fracture position is the weaker C90

Figure 6. Number of carbon-containing organic fragments at different temperatures. (a) Wiser, (b) HQL, and (c) GJL.
and the C60 that are connected to the naphthene and then combine with *H to form C2H2.

3 Cycloalkane connecting the aromatic ring is opened and broken by heating, C76, C136, and methyl fall off, and then, the methyl and a *H fall off, forming a triple bond to generate C2H2.

There are two main paths for CO2 to evolve from the corresponding functional groups:

1 CO2 is produced by decarboxylation. The –COOH on the aromatic ring connected with thiophene is gradually destroyed with the temperature rise, and the *H is removed. After that, the structure becomes unstable and further decarboxylation occurs to generate CO2. This result has been confirmed by related studies.

2 The methyl group on the aromatic ring falls off and loses a *H and then combines with two hydroxyl which lose *H to form CO2. The path occurs in the simulation of the HQL model and GJL model.

4. CONCLUSIONS
Based on the ReaxFF molecular dynamics simulation of three different bituminous coals, we obtained the formation law of molecular fragments with different sizes, the formation law of main inorganic products, and the formation path of main organic products. All results are only responsible for the simulation and have certain universality in theory.

1 With the increase of the temperature, the system potential energy decreases, the endothermic efficiency increases first and then decreases, the reaction becomes violent, the broken degree of coal molecules increases, the fragments of C1−C4 increase, and the gas molecules generated increase. The simulation performance of different bituminous coal models is consistent.

2 In the pyrolysis process, inorganic gas molecules are generated. The oxygen-containing functional groups and hydrogen groups were first broken off and then formed H2O and H2 with the increase of the temperature; therefore, the amount of H2O and H2 increased significantly. H2S is formed after 2000 K, and the sulfur-containing functional groups are almost all broken off with the increase of temperature, while H2S as an
Table 2. Formation Paths of Gases

| Gases   | Serial number | Formation paths |
|---------|---------------|-----------------|
| C₂H₄    | 1             | ![Formation Path 1](image1) |
|         | 2             | ![Formation Path 2](image2) |
|         | 3             | ![Formation Path 3](image3) |
| C₂H₂    | 1             | ![Formation Path 4](image4) |
|         | 2             | ![Formation Path 5](image5) |
|         | 3             | ![Formation Path 6](image6) |
| CO₂     | 1             | ![Formation Path 7](image7) |
|         | 2             | ![Formation Path 8](image8) |
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