Simulation of Lignite Pyrolysis and Gasification in Equilibrium

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The development of lignite pyrolysis and gasification technology is helpful to improve the utilization value of lignite which is abundant in China. From the point of view of mass and energy balance, simulation of lignite pyrolysis and gasification process in equilibrium were conducted. The effects of moisture and ash in lignite and fixed carbon retention rate on reaction results were systematically discussed. The results were shown that yield and quality of gas and coke yield decreased with the increase of moisture in lignite. With the increase of ash content, the coke yields increased, the carbon content of coke decreased and the coke quality became poor. As the retention rate of fixed carbon increased from 50% to 100%, both coke yield and quality increased, the carbon content of coke rose from 47.04% to 94.09% and coke yield rose from 88.84% to 94.09%.

Keywords: Lignite; Equilibrium; Pyrolysis and Gasification; Coke; Gas.

1. Introduction

Lignite resources in China are abundant [1], but most of them are burned as fuel or discarded directly. Lignite, as a low rank coal, has high moisture, high volatile content and low calorific value [2,3]. It’s hard to store for characteristic of easily oxidized and spontaneous combustion. As the consequence of high transport cost, the upgrading of lignite by pyrolysis and gasification is essential [4–6]. The technology of lignite pyrolysis and gasification is an efficient and less polluting utilization because that can not only solve the problem of lignite utilization process, but also get coke, tar, gas and other coal based products. From the beginning of the 1970s, a variety of lignite pyrolysis upgrading process [7–9], in which equipment and product were studied, were developed. In this paper, from the point of view of mass and energy balance, simulation of lignite pyrolysis and gasification process in equilibrium were conducted. The effects of moisture and ash in lignite and fixed carbon retention rate on reaction results were systematically discussed.
2. Calculation Methods

On the base of lignite properties analysis data, Gibbs free energy minimization method is used to predict the lignite gasification products [10,11]. In a certain temperature and pressure, the solution of equation \( G = \sum n_i G_i \) can be obtained when the value of Gibbs free energy(G) of the system is minimum. The obtained gas components are used for calculating mass and energy balance in lignite gasification equilibrium [12~15]. The gas outlet temperature is set as 750°C; there is no tar; The reactor heat dissipation is set as unchanged and air temperature is 25°C.

Energy balance equation as in Eq.(1).

\[
Q_1 + Q_2 + Q_3 = V_1 \left( Q_4 + Q_5 + Q_6 \right) + m_1 \left( Q_7 + Q_8 \right) + Q_9
\]  

\( Q_1 \) is the sensible heat of lignite(ar), kJ/kg(ar); \( Q_2 \) is the sensible heat of lignite(ar), kJ/kg(ar); \( Q_3 \) is the sensible heat of air of lignite(ar), kJ/kg(ar); \( V_1 \) is gas yield, m³/kg(ar); \( Q_4 \) is the sensible heat of dry gas, kJ/m³; \( Q_5 \) is higher calorific value of dry coal gas, kJ/m³; \( Q_6 \) is the heat of steam in coalgas, kJ/m³; \( Q_7 \) is the heat value of coke, kJ/kg(coke); \( Q_8 \) is the sensible heat of coke, kJ/kg(coke); \( Q_9 \) is heat loss, kJ/kg(ar).

The simplified form of higher heating value of dry coalgas as in Eq. (2).

\[
Q = \left( 12.62 \times CO + 12.75 \times H_2 + 39.82 \times CH_4 + 70.06 \times C_2H_4 \right) / 100
\]  

\( Q \) is higher heating value of dry gas, MJ/m³; \( CO, H_2, CH_4 \) and \( C_2H_4 \) present volume fraction respectively in dry gas.

3. Results and Discussion

3.1 Material properties

Ultimate analysis and proximate analysis of lignite are shown in table 1.

<table>
<thead>
<tr>
<th>Ultimate analysis</th>
<th>Proximate analysis</th>
<th>( Q_{net,ad}/(kJ/kg) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( %_{ad} )</td>
<td>( %_{ad} )</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>H</td>
<td>O</td>
</tr>
<tr>
<td>71.5</td>
<td>4.94</td>
<td>22.2</td>
</tr>
</tbody>
</table>

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3.2 The effects of moisture and ash

Gas components changes with the moisture content in lignite are shown in Figure 1. As the moisture content increases, N\textsubscript{2} and CO\textsubscript{2} proportions in gas increase, but CO, H\textsubscript{2}, CH\textsubscript{4} and C\textsubscript{2}H\textsubscript{4} decrease. As is shown in Figure 2, when moisture content is 5%, gas calorific value reaches 7.485MJ/m\textsuperscript{3}. As moisture content increases to 89%, gas calorific value decreases to 0, and gasification efficiency is from 64.8% down to 0. Carbon content of coke keeps invariant but coke yield is from 19.53% down to 2.26%.

Figure 1. Mar vs gas components.

Figure 2. Reaction changes with Mar.
Figure 3 presents reaction changes with the moisture content, when the moisture content is 25% and the retention rate of fixed carbon is 90%. As ash increases, coke yield increases from 15.42% to 35.09%, the carbon content of coke decreases from 84.68% to 64.8%. The results indicate that coke yield increases but the quality of coke becomes worse for higher ash content. Gas calorific value decreases from 6.812 MJ/m$^3$ to 5.679 MJ/m$^3$.

Figure 3. reaction change with ash.

Figure 4. Reaction changes with fixed carbon retention rate.

Figure 4. Reaction changes with fixed carbon retention rate.
3.3 The effects of retention rate of fixed carbon

Figure 4 presents reaction changes with the retention rate of fixed carbon, when the moisture content is 25% and ash content is 90%. The retention rate of fixed carbon means percentage of fixed carbon which was retained in coke. As the retention rate of fixed carbon is from 50% up to 100%, coke yield rises from 21.48% to 42.73%, and the carbon content of coke increases from 88.84% to 94.09%. The results indicate that coke yield and the carbon content of coke can be raised through improving the retention rate of fixed carbon, which can be implemented by optimizing process to avoid fixed carbon burning. Gas calorific value is from 6.812 MJ/m³ down to 5.679 MJ/m³. Gasification efficiency decreases from 50.97% to 16.81%.

4. Conclusions

In this paper, from the point of view of energy and mass balance, simulation and analysis of lignite pyrolysis and gasification in equilibrium were conducted. The results are as follows:

(1) Gasification efficiency decreases with increase of moisture content, ash content and the retention rate of fixed carbon. When moisture content is 5%, gas calorific value is 7.485MJ/m³. As moisture content increases to 89%, Coalgas Calorific value decreased to 0, and gasification efficiency is from 64.8% down to 0. Coke yield is from 19.53% down to 2.26%, but carbon content of coke keeps invariant.

(2) Coke yield increases with ash content and increase of retention rate of fixed carbon, but decreases with the moisture content increasing. The carbon content of coke decreases with ash content increasing. As the retention rate of fixed carbon is from 50% up to 100%, coke yield rises from 21.48% to 42.73; the carbon content of coke increases from 88.84% to 94.09%; gas calorific value is from 6.812 MJ/m³ down to 5.679 MJ/m³; gasification efficiency decreases from 50.97% to 16.81%.

Acknowledgements

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References

