Simulation of Coal Water Slurry Gasification based on Aspen Plus

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Abstract. Based on the description of the gasification process, the suitable thermodynamic model and the components involved in the simulation are selected, and the Aspen Plus is used to analyze the water-coal slurry gasifier. The simulation results are compared with the design data, and the influence of different parameters on the gasification of coal water slurry is studied, and the causes of different effects is analyzed.

1. Introduction
Coal gasification technology, as an important part of chemical production, can replace oil and natural gas in many fields, and has contributed to saving resources and alleviating the increasingly prominent energy and environmental problems. In recent years, the pressurized gasification of coal-water slurry with advanced airflow bed reactor has become one of the mainstream of coal gasification technology, and has also received more and more attention in the development of modern coal chemical technology [1]. At present, there have been some studies on the gasification of water coal slurry [2-4]. Aspen Plus software will be used to simulate the coal water slurry gasifier to study and analyze the different factors affecting the coal water slurry gasification technology. Based on a semi-coke syngas project, the GE coal slurry gasifier model is completed. The main operating conditions of coal slurry gasification, such as oxygen-coal ratio, coal slurry concentration, temperature and pressure, are analyzed by using the model.

2. Description of gasification process
GE coal water slurry gasifier is a pressurized gasification technology with coal water slurry as raw material and oxygen as gasifier. The coal slurry enters the gasifier through the gasification burner at the top of the gasifier after pressurized by the raw material pressure pump. In the combustion chamber, the coal slurry reacts with oxygen at 7.5 MPa, about 1400℃ to form CO, H2, CO2, H2O and a small amount of CH4, H2S, COS and trace NH3, HCOOH.

Crude syngas from the gasification reaction chamber directly enters into the gasifier cooling chamber through the tube to complete the syngas cooling washing, the synthesis temperature of the cooling chamber about 250℃. Carbon black in coarse synthetic gas is mostly removed in the cooling chamber, and the temperature from slag water outlet (N1) to slag breaking machine can reach about more than 1000℃. The outer wall of the shell of the gasifier is equipped with a wall temperature
monitoring system, and the temperature of the reaction chamber is measured by a thermocouple extending into the refractory material. When the temperature of a certain area (0.1 ms) of the outer wall of the reaction chamber reaches about 360℃, the high temperature alarm. Since the syngas contains a small amount of H2S gas, in order to prevent wet H2S corrosion, the temperature of the outer wall of the gasifier should not be less than 225℃, so as to avoid the dew point corrosion caused by the condensation of the inner wall. The structure of gasifier is relatively simple, with refractory brick as lining. High temperature syngas and molten ash directly erode the refractory lining, so the lining life cycle is limited, generally 1~2 years need to be replaced[5-7].

3. Gasifier process simulation technology

3.1. Thermodynamic model
Coal gasification is the reaction of high temperature, high pressure hydrocarbons and gas mixtures such as CO、H2, and most of the gases produced by the reaction are light gases such as CO、H2、CO2、H2O or hydrocarbons. So the RK-Soave equation is suitable to be used in this simulation to calculate the thermodynamic properties of the matter in the gasification process of water coal slurry[8].The coal gasification process is a complex reaction at a high temperature and high pressure, the process involves a lot of components, and the Aspen Plus provides a better treatment for coal and ash. The conventional components involved in the simulation of coal gasification process are H2O、N2、O2、NO2、NO、S、C、SO2、SO3、H2、NH3、COS, etc. The non-conventional component solid coal is the COAL, ash is ASH, selected component type is Nonconventional.

3.2. Process simulation
The simulation of gasifier mainly includes the pressurized transportation of coal slurry, coal cracking, gasification of coal water slurry and so on. The specific process is as follows: water and coal are mixed through mixer to obtain coal water slurry flow strands S1; and then pressurized by pump to reach the required gasification pressure 6.5 MPa, pressurized coal water slurry flow strands S2; the pressurized coal water slurry enters the pyrolysis unit of the gasifier, according to the conservation of elements, all unconventional solid groups are divided into conventional components. the conventional single mass components of coal water slurry after pyrolysis are divided into flow strands coal, and the pyrolysis heat is transferred to the later gasification simulation reactor to achieve the required temperature of 1350℃ for coal gasification; then the raw coal slurry is mixed with oxygen to simulate the gasification reaction in the Gibbs reactor.

PRODUCTS is the last product airflow. The specific simulation process is shown in Figure 1, coal water slurry gasifier process simulation process:

![Fig.1 Process simulation of CWS gasifier](image)

The coal cracking module does not need to know the kinetic equation of the reaction, but simply gives the stoichiometric number of the conventional components after coal cracking. The simulation uses Rstoic module to decompose coal into H2O、N2、O2、S、H2、C、Ash and other components, and at the same time, the pyrolysis heat is transmitted to the reaction unit.
Meanwhile, industrial analysis (Proxanal), elemental analysis (Ultanal), sulfur analysis (Sulfanal) of coal are performed within this unit module.

Then the cws enter the RGibbs reactor module for simulation. RGibbs does not need to specify the stoichiometric coefficient of the reaction or kinetic parameters, only need to specify the product. RGibbs can calculate the chemical equilibrium between the conventional solid component and the fluid, the unconventional solid ASH is regarded as the inert component does not participate in the equilibrium calculation. Simulations specify that the outlet components are \(H_2\), \(CO\), \(CO_2\), \(H_2S\), \(COS\), \(N_2\), \(HCl\), \(O_2\), \(H_2O\), \(NH_3\), ARGON, as well as unreacted carbon. Finally, by solving a series of nonlinear mathematical programming problems, the equilibrium state of the system in the Gibbs free energy is obtained, and the gasification syngas composition is obtained.

3.3. Testing of models
Comparing the Aspen simulation results with the design data, we can get the comparison results of table 1, the composition of syngas dry base.

| CO/\% | H_2/\% | CO_2/\% | CH_4/\% | Ar/\% | N_2 and others/\% | H_2S+COS/\% |
|-------|--------|---------|---------|-------|-----------------|-------------|
| Simulated data | 49.37 | 30.36 | 19.45 | 0.0062 | 0.134 | 0.4765 | 0.209 |
| Design data | 50.23 | 30.7 | 18.24 | 0.0300 | 0.130 | 0.4500 | 0.220 |

By comparing the simulation data with the design data, it can be seen that the simulation results are basically correct, which can be used to describe the gasification reaction of water coal slurries, and can be used to investigate the influence of operation parameters on the results of water coal slurry gasification reaction.

4. Effect of operating parameters on gasification performance

4.1. Effect of oxygen-coal ratio on gasification of water-coal slurry
When studying the influence of oxygen-coal ratio on gasification, other conditions should be kept constant, and the composition of syngas should be studied by changing the oxygen-coal ratio. The oxygen-coal ratio in the original simulation data is close to 1, and the comparison results are shown in Table 2, the effect of oxygen-coal ratio on the gasification results of water-coal slurry.

| oxygen-coal ratio | H_2/\% | CO/\% | CO_2/\% | H_2O/\% |
|------------------|--------|-------|---------|---------|
| 0.9              | 16.00  | 25.5  | 8.88    | 49.22   |
| 1.0              | 15.12  | 24.59 | 9.69    | 50.2    |
| 1.1              | 13.42  | 22.2  | 12.67   | 51.29   |

By studying, it is found that the increase of oxygen coal ratio will make the reaction intense. Carbon and oxygen combustion in coal water slurry will increase the \(CO_2\) content. The conversion of hydrogen and oxygen to water vapor also increases. When the oxygen coal ratio decreases, the coal will mainly undergo pyrolysis reaction during gasification. Therefore, with the increase of oxygen-coal ratio, the content of \(H_2\) and \(CO\) decreases, and the content of \(CO_2\) and \(H_2O\) increases.

4.2. Effect of coal water slurry concentration on coal water slurry gasification
In the study of the effect of coal water slurry concentration on gasification, other conditions should be kept constant, and the composition of syngas should be studied by changing the concentration of coal.
water slurry. The concentration of cws in the original simulation data was 62%. The comparison results are shown in Table 3, the effect of coal water slurry concentration on the gasification results of coal water slurry.

Table 3 Influence of CWS concentration on gasification results of CWS

| CWS concentration | H2/%  | CO/%  | CO2/% | H2O/% |
|-------------------|-------|-------|-------|-------|
| 60                | 16.28 | 22.70 | 10.11 | 50.51 |
| 62                | 15.12 | 24.59 | 9.69  | 50.2  |
| 64                | 14.93 | 26.35 | 9.26  | 49.06 |

Through the study, it is found that the concentration of coal water slurry increases, the content of carbon component increases, and the reaction with oxygen produces more CO, so the CO concentration in the outlet syngas increases and the CO2 content decreases. On the other hand, the content of H2 and H2O in the outlet syngas decreases because of the decrease of water content and the decrease of the content H of components in the gasification raw material.

4.3. Effect of temperature on gasification of coal water slurry

When studying the effect of temperature on gasification, other conditions should be kept constant, and the composition of syngas should be studied by changing the gasification temperature. Gasification temperature is 1350℃ in the original simulation data. The comparison results are shown in Table 4, the effect of gasification temperature on the gasification results of water coal slurry.

Table 4 Influence of gasification temperature on gasification results of CWS

| Temperature/℃ | H2/%  | CO/%  | CO2/% | H2O/% |
|---------------|-------|-------|-------|-------|
| 1250          | 16.28 | 22.70 | 10.11 | 50.51 |
| 1350          | 15.12 | 24.59 | 9.69  | 50.2  |
| 1450          | 14.93 | 26.35 | 9.26  | 49.06 |

The study found that the gasification temperature increased, the content of effective gas H2, CO decreased, while the content of CO2 and H2O increased, mainly because the gasification temperature increased, C, H components reacted violently with oxygen to produce more CO2 and H2O, while the reaction was endothermic, the temperature increase equilibrium shifted to the right, so the content of CO components decreased.

4.4. Effect of pressure on gasification of coal water slurry

When studying the influence of pressure on gasification, we should ensure that other conditions remain unchanged, and study the composition of syngas by changing the gasification pressure. Gasification pressure was 6.5 MPa in the original simulation data. The comparison results are shown in Table 5, the effect of pressure on the gasification results of water coal slurry.

Table 5 Influence of gasification pressure on gasification results of CWS

| Pressure/MPa | H2/%  | CO/%  | CO2/% | H2O/% |
|--------------|-------|-------|-------|-------|
| 6.0          | 15.12 | 24.59 | 9.69  | 50.2  |
| 6.5          | 15.12 | 24.59 | 9.69  | 50.2  |
| 7.0          | 15.12 | 24.59 | 9.69  | 50.2  |

The results show that the CO, H2, CO2 content is almost constant with the increase of gasification pressure, but the CH4 content will increase. This is mainly because the raw coal has been cracked in the cracking unit during the simulation process, so it is considered that the components entering the combustion chamber are all gas phase, which is close to the constant volume reaction. However, in the actual production process, the reaction proceeds in the direction of volume reduction with the pressure increasing, and the content of solid gas components will be slightly reduced [9-10].
5. Conclusions

(1) A model of coal-water slurry gasifier was established by using Aspen Plus. The simulation results are in good agreement with the design data.

(2) The effects of oxygen-coal ratio, coal-water slurry concentration, gasification temperature and gasification pressure on the components of crude syngas were analyzed. The results show that the effective gas composition decreases but the CO\textsubscript{2} content increases when the ratio of oxygen to coal increases; the higher the concentration of coal water slurry, the higher the CO content of the effective gas composition but the lower the H\textsubscript{2} content; the higher the gasification temperature, the higher the CO\textsubscript{2} and H\textsubscript{2}O content, the lower the effective gas content; the gasification pressure has little effect on the composition of natural gas, but the higher the pressure is, the higher the methane content in natural gas is. It has certain guiding significance for the research of coal water slurry gasifier.

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