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The Thermal Performance Calculation and Analysis of High Temperature Coal Gasifier

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Abstract: High temperature and high pressure entrained flow coal gasification technology is the key technology of coal utilization, and the chemical and physical properties of coal and coke have an important impact on the thermal performance of coal gasification reaction. Based on the research and analysis of the physical and chemical processes of drying, hydrolysis, gasification and combustion in the process of coal gasification, this paper establishes the chemical equilibrium equation of gas composition by using the method of material balance and heat balance, calculates the indexes of coal gasification process, such as carbon conversion rate, cold gas efficiency, specific coal consumption, specific oxygen consumption, and probes into the operation pressure, specific energy consumption, specific energy consumption. The effects of operating temperature, oxygen coal ratio and steam coal ratio on gasification characteristics, such as coal gasification efficiency, coal gas yield and carbon conversion, provide theoretical guidance for the application of high temperature and high pressure coal gasification technology.

1. Introduction

Coal gasification refers to the production of industrial fuel gas, civil fuel gas and chemical feed gas with coal as raw material under the action of catalyst. It is one of the most important ways to use coal resources cleanly and efficiently, and is the key technology and important link of many energy high-tech. At present, the mature and industrialized gasification methods include fixed bed gasifier, mixed gas producer, water gas producer, two-stage gas producer and pressurized gasifier. Winkler gasification of liquidized bed gasification and K-T gasification of entrained flow gasification process [1].

With the development of coal gasification technology, large-scale, high-temperature and high-pressure coal gasification technology has become the development trend of clean coal technology. The selection of coal gasification technology is the key to the success of oil to coal. Coal water slurry gasification technology and dry powder coal gasification technology have been used as the preferred technology [2]. After long-term development, introduction, digestion and absorption, important progress has also been made in the research and development of coal gasification technology in China. However, the entrained flow coal gasification technology of East China University of Science and Technology, the atmospheric intermittent liquidized bed coal gasification technology of Jiangsu University of Science and Technology, and the ash agglomerating fluidized bed pulverized coal gasification technology developed by Shanxi Institute of Coal Chemistry, Chinese Academy of Sciences, are prevalent in the high price of gasifier devices, low coal conversion rate.

The gasification reactivity of coal at high temperature and high pressure is one of the most important factors affecting the efficiency of high temperature coal gasification. The operating pressure and temperature of entrained flow gasifier are usually about 1300 to 1700 at atmospheric pressure. The influence of the chemical and physical properties of coal and coke on the reactivity of coal gasification has been widely studied and applied [3], but the kinetic data and research conclusions therein lack effective pertinence for coal gasification at higher temperatures and pressures. The coal gasification characteristics of typical coals under high-temperature and high-pressure atmosphere are urgently needed to provide strong theoretical and data support for the development of coal gasification technology.

2. Coal Gasification Principle

The gasification process of coal is a thermochemical process. It takes coal or coal char as raw material, oxygen, water vapor or hydrogen as catalyst, and converts raw coal from solid fuel to gas fuel through partial oxidation reaction under high temperature [4,5]. Technically, the coal gasification process often includes the purification process of gasification gas, that is, the process of removing impurities such as ash and sulfur in the gasification gas through purification equipment to obtain clean and easy to transport gas fuel. In essence, the coal gasification process is a process in which the coal is converted into gas fuel with certain potential chemical energy through partial oxidation reaction by controlling the oxygen supply.

The gasification reaction in the gasifier is mainly the reaction of carbon in coal with oxygen, water vapor, carbon dioxide and hydrogen in the gasifier, as well as the reaction between carbon and products and products. It has gone through several processes of drying, hydrolysis, gasification and combustion, as shown in Figure.1.

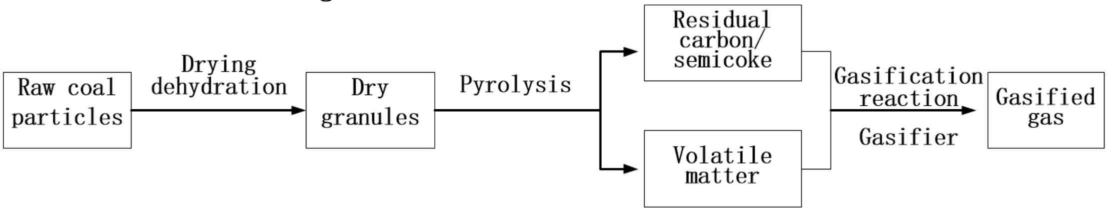

Figure 1: Diagram of coal gasification process

During the whole process, when the wet coal is added to the gasifier, the water in the coal evaporates due to the heat exchange between the coal and the hot gas flow. When the temperature of coal particle rises to 350, the coal pyrolysis reaction begins, and volatile matte is separated. The gasification reaction of coal is carried out under anoxic condition, so the main products of coal gasification reaction are combustible gases CO, H_2 and CH_4, and only a small part of C is completely oxidized to CO_2. In addition, other elements in coal, such as sulfur and nitrogen, will also react with the gasification agent to generate H_2S, COS, N_2 and NH_3 in a reducing atmosphere.

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3. Chemical Equilibrium Model of Coal Gasification

3.1. Calculation Model at Given Temperature

The calculation purpose of coal gasification process is to determine various gasification indexes when a certain coal is used as raw material, and its basis is material balance equation and heat balance equation. It is required to calculate the gas component share under the following conditions of gasifier feed boundary, coal industry analysis and element analysis data, as shown in Table 1.

Table 1: Feed Boundary of GasifierItem

	Value /(t d^{-1})	Temperature/°C	Pressure/MPa
Coal feeding quantity	2897	80	/
Oxygen consumption of gasifier	2390	150	3.85
Steam volume	343	300	4.75
Nitrogen delivery	63	80	4.75

The materials input into the gasifier are raw coal and gasifier, and the materials output from the gasifier are raw gas, tar, entrainment and ash. In a certain period of time, the quality of both is equal. As the atoms of each element will not change during the gasification process, whether it is the flow of materials or the process of pyrolysis and gasification, the mass of each element input into the gasifier system and the mass output from the system will not change within a certain period of time.

The coal gasification system is an open system for maintaining mass balance. Phase equilibrium exists between different phases of substances participating in the reaction in the system. The same substance existing in different phases is a different component. According to the second law of thermodynamics, chemical reaction always goes in the direction, when the enthalpy function reaches the maximum value and Gibbs function reaches the minimum value, the system reaches equilibrium [6,7]. If the coal gasification pressure is known and the coal gasification temperature is assumed to be determined, the following can be obtained according to the full differential equation of Gibbs function.

When the coal gasification reaction system under constant temperature reaches the equilibrium state, the Gibbs function reaches the minimum value, which is the chemical equilibrium state. In the process of coal gasification, the minimum value of Gibbs function is obtained when the components in equilibrium state are required to meet the element conservation equation. Under the condition that the element conservation equation is satisfied, this paper applies the method of Lagrange multiplier to find the extreme value to find the minimum value of the Gibbs function of the system.

$$\begin{cases} \min(G(T,P,\mathrm{n})) \\ An = b \end{cases} = \begin{cases} \min\left(\sum_{i=1}^{N} n_i \mu_i\right) \\ \sum_{i=1}^{N} a_{ki} n_i = b_k \end{cases} \qquad k=1,\ 2,\ 3,\ \ldots,\ M \tag{1}$$

$$\ell(n,\ \lambda) = \sum_{i=1}^{N} n_i \mu_i + \sum_{k=1}^{M} \lambda_k \left(b_k - \sum_{i=1}^{N} a_{ki} n_i \right) \tag{2}$$

The specific iteration process aims to meet the chemical equilibrium conditions, so that the results of each iteration meet the conservation conditions of components, and the method of establishing the coal gasification reactor model. In view of the situation that there is no operating temperature in the feed boundary conditions, the program calculates the respective iteration step size. The simulation analysis determines the reaction temperature and component share based on the coupling method of adiabatic gasification conditions and non-adiabatic gasification conditions.

3.2. Calculation Method under Uncertain Gasification Temperature

For the iterative method of gas composition under the determined temperature cannot be applied to the case where only the operating pressure is used in the calculation of boundary conditions without the temperature conditions being given, it is necessary to find a method to simultaneously solve the gasification temperature and composition, that is, the gasification temperature is coupled with the gas component share, and a gasification temperature corresponds to the unique gasification component share.

Adiabatic gasification temperature is the average temperature of gas when the furnace wall is in an adiabatic state and the gasification reaches equilibrium. Under adiabatic gasification conditions, the thermal effects obtained from gasification are used to heat the products. According to chemical thermodynamics, the sum of standard heat of formation and sensible heat of reactants is equal to the sum of standard heat of formation and sensible heat of products. Standard heat of formation in reactants oxygen and nitrogen are simple substances, and the standard heat of formation is zero. The standard heat of formation of elements in coal is zero, the standard enthalpy of formation of water is -241.82J mol-1, and the standard heat of formation of ash can be eliminated in calculation.

From the above analysis, when the mass flow rate, temperature, gasification pressure and component share in the balance system of the feed are given, the relationship between the constant pressure heat capacity and temperature can be obtained as follows.

$$F(T_{\text{II}}) = (Q_{SX})_1 + (Q_{SX})_2 - constant = 0 \tag{3}$$

Then, Newton Raphson method can be used to calculate the gasification temperature corresponding to the component fraction at this time. The flow chart for solving the adiabatic gasification temperature is shown in Figure 2.

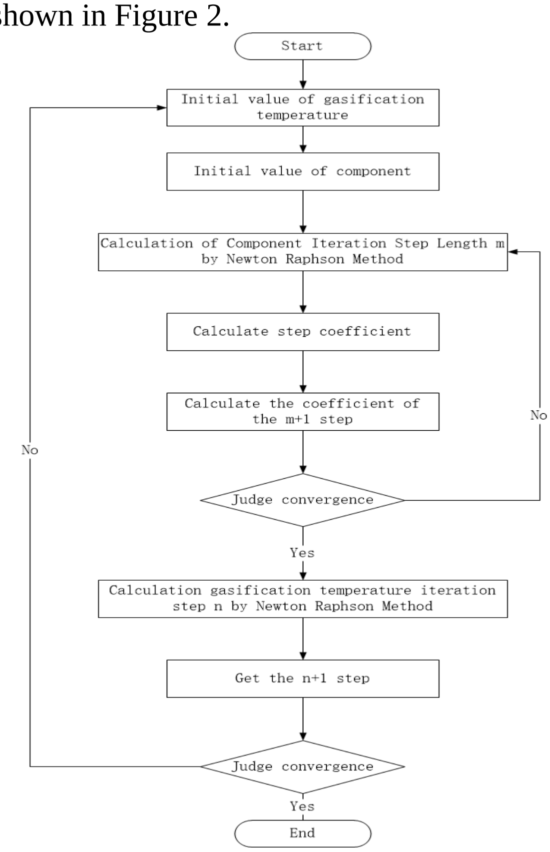

Figure 2: Flow chart of gas composition algorithm under uncertain gasification temperature

4. Calculation and Analysis of Thermal Performance of Coal Gasifier

4.1. Calculation of Gasification Index

According to the calculation model of the raw gas component share of the gasifier under different conditions, the raw gas component share obtained under the given feed boundary conditions in Tab.1 is shown in Table 2, and the adiabatic gasification temperature is 1892.37 K.

Table 2: The share of raw gas components and the amount of their substances

Component	Colume/%	Substance/kmol
CO	59.932	6104.7642
CO_2	2.66	270.9686
COS	0.082	8.3553
CH_4	2.931	298.4603
H_2S	0.52	52.9753
H_2	28.87	2940.8486
H_2O	1.73	176.2317
N_2	3.24	330.0421

The purpose of coal gasification process calculation is to determine various gasification indicators when a certain coal is used as raw material for gasification. These indicators are not only the main technical and economic indicators of coal gasification production, but also the original basis for public welfare design and operation. The gasification indexes of coal gasification process mainly include gas composition and calorific value, gas yield, gasification intensity, gasifier consumption, gasification efficiency and thermal efficiency. The calculation results of coal gasification process characteristic indexes are shown in Table 3.

Table 3: Coal Gasification Process Characteristic Indexes

Gasification parameters	Calculated value
Gasification pressure/Mpa	3.85
Gasification temperature/K	1892.37
Carbon conversion rate/%	97.19
Gas efficiency/$m^3 \cdot kg^{-1}$	1.9
Gasification rate/%	85.2

4.2. Simulation Analysis of Thermal Performance of Coal Gasifier

4.2.1. Effect of Gasification Temperature

Keep other gasification parameters unchanged, calculate the gas composition at the gasification temperature of 600K, 700K, 800K, 900K, 1000K, 1100K, 1200K, 1300K, 1400K, 1500K, 1600K, 1700K and 1800K respectively, as shown in Figure 3 and Figure 4.

It can be seen from Figure 3 and Figure 4 that when the operating pressure is constant, with the increase of gasification temperature, the mole fraction of unreacted carbon in the reaction system decreases rapidly, and the volume fraction of CO increases. However, the increase of gasification temperature decreases the equilibrium coefficient of water gas reaction, resulting in the decrease of CO_2 volume fraction, and CO still keeps increasing. When the gasification temperature is higher than 1300K, the carbon conversion rate tends to 100%. As the volume fraction of CO keeps increasing monotonously, the gasification efficiency will also increase monotonously, and then tends to be stable due to the slowing down of CO increase rate. Therefore, to obtain good gasification efficiency, it is necessary to increase the gasification temperature. Although the increase of operating pressure will improve the gasification intensity and production capacity, it will also affect the volume fraction of CO.

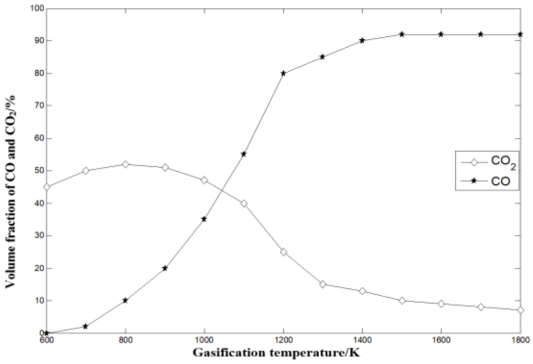

Figure 3: Effect of Temperature on Volume Fraction of CO and CO_2

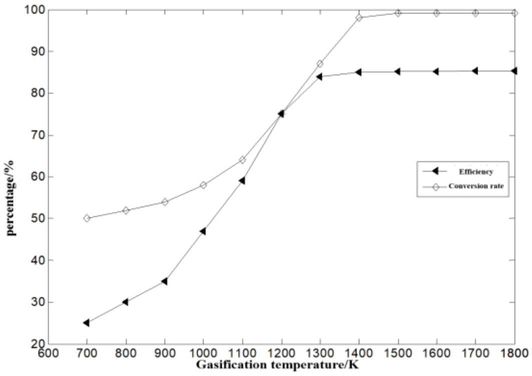

Figure 4: Influence of Temperature on Carbon Conversion and Gasification Efficiency

4.2.2. Effect of Oxygen Coal Ratio

Under the condition that the amount of coal and steam is unchanged, change the amount of oxygen fed into the furnace, calculate with the prediction program, and obtain the change state of each component share under different oxygen coal ratio, as shown in Figure 5.

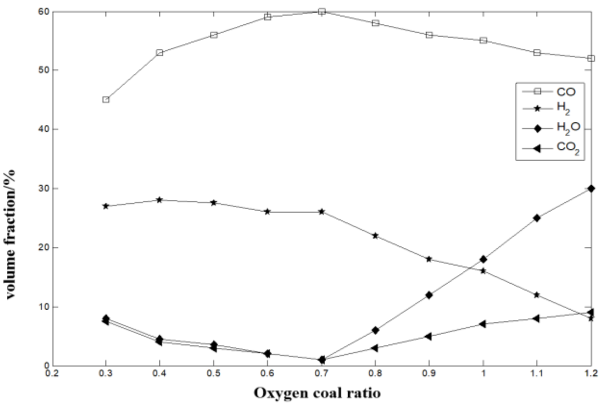

Figure 5: Effect of oxygen coal ratio on volume fraction of H_2, H_2O, CO and CO_2

It can be seen from Figure.5 that at low oxygen coal ratio, due to insufficient oxygen, a large number of single value carbon do not react. The system reduction system has low gasification temperature and low reaction rate of steam decomposition reaction, so the volume fraction of H2, CO and CO_2 is small. When the oxygen supply is increased and the oxygen coal ratio is increased, the single value carbon in the system reacts with oxygen to generate a large amount of CO, and a large amount of heat is released at the same time, thus improving the reaction rate of steam decomposition reaction. Therefore, the volume fraction of CO and H_2 gradually increases, and the volume fraction of water vapor gradually decreases. As the gasification temperature increases, the equilibrium constant of the water gas reaction decreases, and the equilibrium moves to the left, resulting in a decrease rate of H_2 greater than that of CO, and an increase rate of H_2O greater than that of CO_2.

4.2.3. Effect of Steam Coal Ratio

Under the condition that the amount of coal and oxygen is unchanged, change the amount of steam fed into the furnace, calculate with the prediction program and method, and obtain the change of each component share under different steam coal ratio, as shown in Figure.6 and Figure.7.

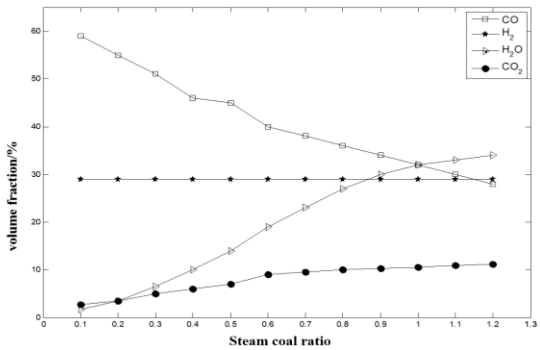

Figure 6: Effect of Steam coal Ratio on H_2, H_2O, CO and CO_2

In the original balance, adding water makes the water gas reaction equation (4) move to the right, the volume fraction of CO decreases with the increase of steam coal ratio, CO2 increases with the increase of steam coal ratio, and the volume fraction of H_2 basically remains unchanged.

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (4)$$

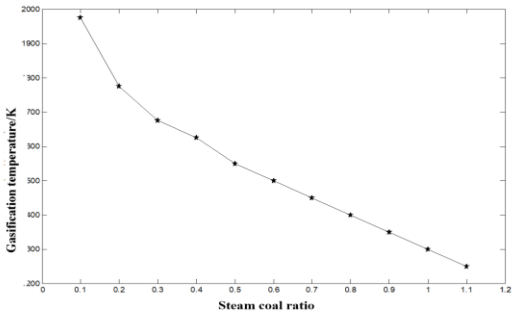

Figure 7: Effect of steam coal ratio on gasification temperature

It can be seen from Figure 6 that when the water vapor increases excessively, some of the water vapor does not participate in the gasification reaction. This part of the water vapor is called the cooling medium of the raw gas, which causes the gasification temperature to drop rapidly. Thus, during the gasification process, the added water vapor or the water in the raw coal reacts with the carbon under high temperature to form a strongly endothermic water gas reaction, which increases the content of CO and H_2 in the gas, controls the furnace temperature not to be too high, and reduces the oxygen consumption. However, when the steam coal ratio is too high, the furnace temperature will be reduced, which will hinder the reduction of CO_2 and the decomposition reaction of water vapor and affect the gasification process. At the same time, due to the consumption of a large amount of latent heat of gasification, the cold gas efficiency will be reduced, so will the content of CO and H_2 in the raw gas.

5. Conclusions

In this paper, based on the principle of material balance and heat balance, a reactor model corresponding to the minimum free energy of the system parameters during reaction balance is established for reaction calculation. The calculation process is developed by coupling adiabatic gasification conditions with non-adiabatic gasification conditions. The program of coal gasification operation temperature and component share is compiled and the simulation results are obtained. The effect of gasification parameters on coal gasification efficiency The influence of gasification characteristics, such as gas yield and carbon conversion rate, has obtained the theoretical basis for the application of high-temperature and high-pressure coal gasification technology.

The analysis results show that increasing the temperature can increase the content of CO and H_2 in the gas, and improve the gasification efficiency, gas yield and carbon conversion; The oxygen coal ratio has a great influence on the gasificationxijinpinh process. The increase of the oxygen coal ratio increases the heat release of combustion reaction, increases the content of CO and H_2 in the gas, thus improving the calorific value of the gas and the conversion rate of carbon. At the same time, the increase of the oxygen content increases the invalid components in the gas; The steam coal ratio has little effect on the volume fraction of H_2 and CO_2.

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