Simulation of co-production system based on coal partial gasification under different reactant gas atmospheres

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Abstract- In order to explore the comparison of coal partial gasification hydrogen-electricity cogeneration systems under different gasification agent atmospheres, based coal partial gasification, including steam cycle power generation and syngas processing for hydrogen production, a hydrogen-electric co-production system and its model of partial coal gasification and semi-coke combustion are constructed, respectively using (H_2O/O_2) and (CO_2/O_2) as gasification reactant gas. The effects of oxygen-coal ratio and carbon conversion on exergy efficiency and syngas composition under different gasification reaction gas atmospheres were studied by Aspen Plus simulation. The exergy efficiency under different gasification agent atmospheres increases first and then decreases with the increase of oxygen-coal ratio and carbon conversion rate. Using (CO_2/O_2) as gasification agent has higher exergy efficiency. The composition of syngas changes little under different oxygen-coal ratios, while the overall content of H_2, CO and CH_4 in syngas will increase with the increase of carbon conversion rate, but the growth rate will continue to decline.

1. Introduction

Coal plays a leading role in China 's fossil energy reserves and consumption. The proportion of this consumption will not change in the next few decades. With the national policy of ' carbon peak, carbon neutralization ', how to use coal grading technology to make coal more efficient and pollution-free is related to environmental protection and energy security[1]. At present, the construction of coal co-production technology is a mainstream research idea, with coal gasification, power generation and chemical synthesis as the main body. Coal gasification can be divided into partial gasification and complete gasification of coal. The partial gasification is separated and treated separately according to the different activities of each component in coal, without pursuing a higher degree of gasification to meet different needs. Coupling steam power generation cycle and syngas treatment technology to build coal partial gasification co-production system. At present, the main gasification reactant gas used for coal partial gasification are air, steam, O_2 and CO_2[2]. Coal pressurized fluidized bed partial gasification technology was proposed by Shanxi Coal Chemical Research Institute[3]. The pressurized fluidized bed gasifier was used as the core, and the gasification atmosphere is (CO_2/O_2). The effects of coal type and initial temperature of gasifier on gasification characteristics were analyzed. The coal partial gasification combined power generation cycle proposed by Zhejiang University, coal and air/steam gasification reaction, gasifier atmospheric operation, build a simple purification unit[4].

For improving the efficiency of coal utilization, improve the efficiency of the cogeneration system, and reduce CO_2 emissions during coal gasification hydrogen production, this paper uses coal partial gasification technology coupled with semi-coke pressurized oxy-fuel combustion technology to propose a coal partial gasification co-production system, and uses (H_2O/O_2) and (CO_2/O_2) as gasification reactant gas to be fed into a pressurized circulating fluidized bed gasifier to react with coal. The advantages and disadvantages of different gasification reactant gas and their effects on the exergy efficiency of the system, as well as the effects of oxygen-coal ratio and carbon conversion rate on the exergy efficiency and syngas composition ratio under different gasification reactant gas atmospheres are compared and analyzed. Aspen Plus was used for numerical simulation.

2. System simulation

2.1 System introduction

Fig. 1 is a flow chart of the system being built, using (A) H_2O and O_2; (B) CO_2 and O_2 into the gasifier.

The air separation unit (ASU) provides high concentration oxygen, the steam power generation cycle provides high temperature steam, and the CO_2 capture unit provides CO_2. The coal material enters the pressurized circulating fluidized bed gasifier through the feeder, and

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reacts with the selected gasification agent and desulfurizer at 950 °C to produce gasification products. The gasifier product is separated by the cyclone separator to obtain crude syngas and solid semi-coke. Semi-coke was fed into pressurized circulating fluidized bed combustion furnace. The crude syngas is fed into the syngas purification and reforming unit. After purification and impurity removal, the reforming reaction is used to increase the proportion of H_2 in the synthesis, and the pressure swing adsorption device (PSA) is used to separate H_2 and CO_2, and store H_2 and CO_2 respectively to achieve zero CO_2 emission of the system[5].

The reaction of coal in the gasifier is very complex. Aspen Plus different modules are used to simulate different processes in the gasification process. Mongolian mixed coal is selected as raw material. The proximate and ultimate analysis of Mongolian mixed coal are shown in table 1[6], and the coal intake is set to 72kg/h.

According to the element conservation, the input coal was decomposed into C, H_2, S, O_2, Cl_2, O_2, ASH and the corresponding yield was obtained. The combustion process uses the RGibbs reactor module to obtain gasification products, and then uses the Sep module to simulate the gas-solid separation process.

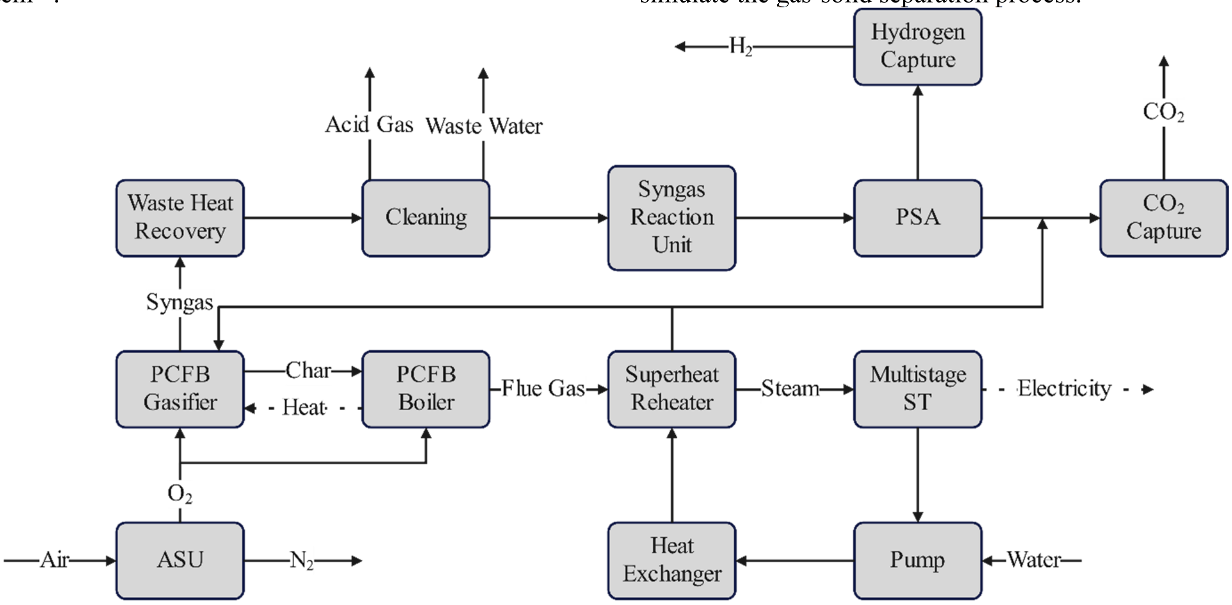

Fig.1 Diagram of coal partial gasification co-production system

Table 1. The proximate and ultimate analysis of Mongolian mixed coal

Ultimate analysis/(wt%)		Proximate analysis/(wt%)	
C_{ar}	65	M_{ar}	0.00
H_{ar}	3.36	A_{ar}	10.00
N_{ar}	0.78	V_{ar}	32.80
S_{ar}	0.36	FC_{ar}	57.21
O_{ar}	20.50	$Q_{net,ar}$/(MJ/kg)	28.54

In the combustion furnace, the semi-coke reacts with oxygen at 2MPa to produce high-temperature flue gas, which is separated by a cyclone separator. The solid waste passes through the medium temperature superheater (MTS) and the low temperature superheater (LTS) to make the water vapor overheat and return to the combustion furnace. The gaseous flue gas generates superheated water vapor through the high temperature superheater (HTS) to enter the steam turbine (ST) for electricity, and then passes through high temperature reheater (HTR), the low temperature reheater (LTR) and economizer to release heat to re-superheat the water vapor for electricity, and finally returns to the steam cycle through the condenser as liquid water. One (37%) of the flue gas at the outlet of the economizer returns to the combustion furnace, and the other flue gas (63%) enters the CO_2 capture unit to store CO_2 after the steps of impurity removal, distillation and pressurization. The superheated water vapor heated by the multi-stage heat exchanger passes through three steam turbines with different pressures in the water vapor cycle to output electricity[7].

For the purification and conversion of syngas, the separation of H_2 and the capture of CO_2, the Selexol technology was used to desulfurize the syngas. The model was simplified to a Sep model for removing H_2S and other acidic gas in the syngas. CH_4 reforming reaction and CO change reaction were used in the reaction unit to convert CH_4 and CO into H_2 and increase H_2 production. Using pressure swing adsorption (PSA) technology, Sep was used to simplify the model, CO_2 was separated and captured, and then H_2 with a purity of 99 % was obtained.

2.2 Methodology

Efficiency is an important index to evaluate performance and efficiency[8]. Table 2 shows the meaning of the parameters in the calculation formula.

From the perspective of conservation of system exergy:

$$Ex_{in} + Ex_{Q,in} + Ex_{W,in} = Ex_{out} + Ex_{Q,out} + Ex_{W,out} \tag{1}$$

After ignoring the kinetic exergy and potential exergy, the logistics is:

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$$Ex = Ex_{ph} + Ex_{ch} \tag{2}$$

$$\overline{Ex}_{ph} = (H_i + H_0) - T_0(S_i - S_0) \tag{3}$$

$$\overline{Ex}_{ch} = \sum y_i * \overline{E^o x}_{ch,i} + RT_0 \sum y_i \, ln y_i \tag{4}$$

$$Ex_{coal} = \overline{E^o x}_{coal} * m_{coal} \tag{5}$$

$$\overline{E^o x}_{coal} = LHV_{coal} * \left(1.0438 + 0.0013\frac{H}{C} + 0.1083\frac{O}{C} + 0.0549\frac{N}{C}\right) + 6.71S \tag{6}$$

Exergy efficiency is calculated as follows:

$$\varepsilon = \frac{Ex_{Hydrogen} + W_{out}}{Ex_{coal} + W_{in}} \tag{7}$$

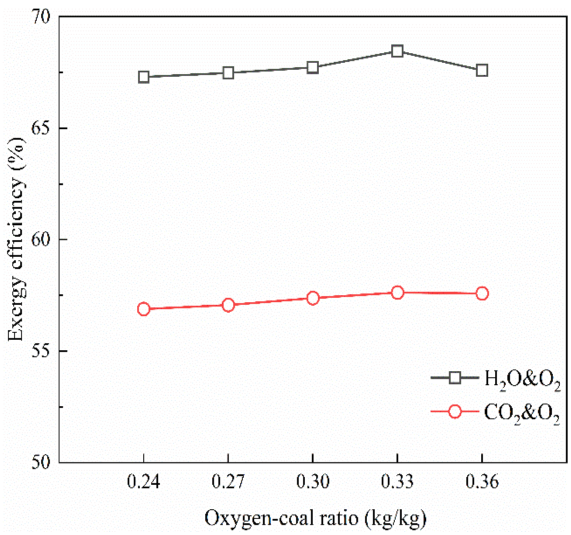
Table 2. Parameter meaning

Parameters	Unit	Meaning
LHV_{coal}	MJ/kg	Lower calorific value of coal
m_{coal}	Kg/s	The coal mass flow
$LHV_{Hydrogen}$	MJ/kg	The lower calorific value of H_2
Ex_{ph}	MW	The physical exergy
Ex_{ch}	MW	The chemical exergy
Ex_{coal}	MW	The exergy of coal
$\overline{Ex}_{ph}$	MW/mol	The physical exergy per mole
$\overline{Ex}_{ch}$	MW/mol	The chemical exergy per mole
$\overline{E^o x}_{ch,i}$	MJ/kmol	The standard chemical exergy value
$\overline{E^o x}_{coal}$	MW/mol	The exergy per mole of coal
ε	%	The exergy efficiency

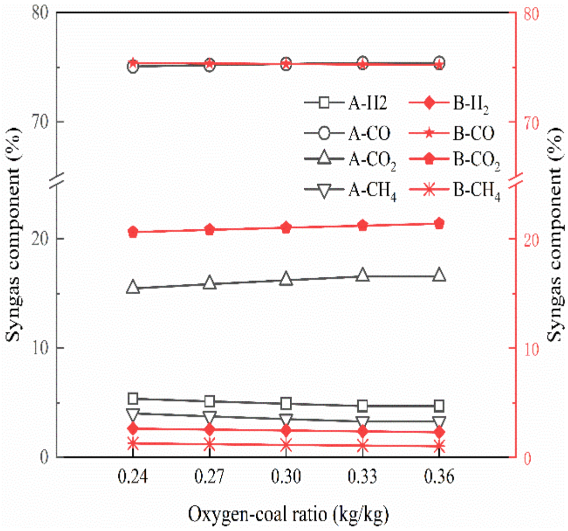
3. Results and Discussions

3.1 The effects of oxygen-coal ratio on system

The ratio of oxygen mass flow rate to coal mass flow rate entering the gasifier is called oxygen coal ratio. Fig.2 (a) shows the variation trend of exergy efficiency of different gasification agent systems with different oxygen-coal ratios. The increase of oxygen-coal ratio makes the exergy efficiency increase first and then decrease. The system using CO_2 and O_2 as gasification agents has higher exergy efficiency under different oxygen coals than the system using H_2O and O_2 as gasification agents. The gasification reaction will become more intense with the increase of oxygen coal ratio, the degree of gasification deepens, and the yield of syngas increases slightly[9]. As shown in fig.2 (b), with the increase of oxygen coal ratio, CO and CO_2 increase slightly, H_2 and CH_4 content decrease, the increase of oxygen in gasifier makes the combustible gas content in syngas decrease, and the calorific value decreases. The increase of oxygen coal ratio increases the oxygen consumption of the system, which requires more extra work input to the system to prepare oxygen, so that the system efficiency increases first and then decreases.



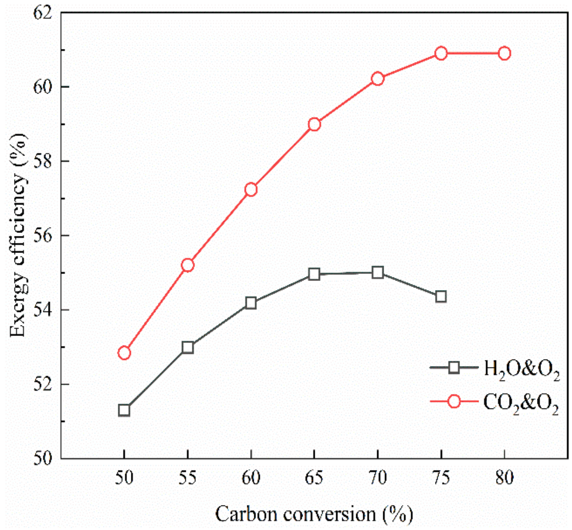
a. The effects of oxygen coal ratio on exergy efficiency.



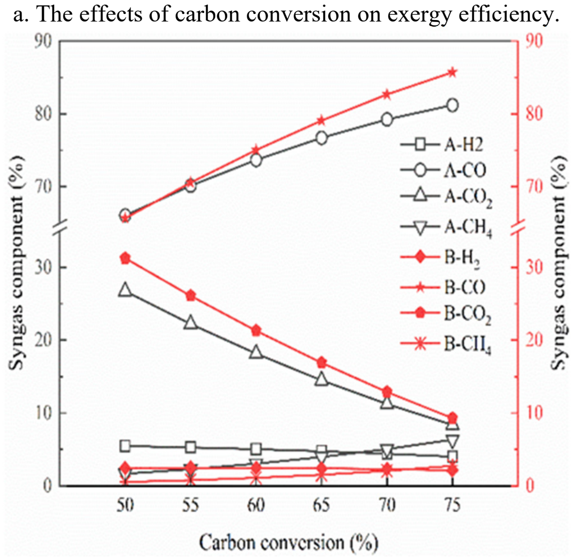
b. The effects of oxygen coal ratio on syngas component.
Fig.2 The effects of oxygen coal ratio on exergy efficiency and syngas component.

3.2 The effects of carbon conversion on system

When the gasification temperature is 950 °C, the gasification pressure is controlled at 2 MPa, and the oxygen-coal ratio is fixed at 0.3, the influence of carbon conversion rate on the exergy efficiency of coal partial gasification system with different gasification agents is analyzed. Fig.3 (a) is the change trend of exergy efficiency. The maximum exergy efficiency is 55.01 % when the carbon conversion is 65 % by using H_2O and O_2, and the maximum exergy efficiency is 60.91 % when the carbon conversion is 70 % by using CO_2 and O_2. The latter system has advantages in exergy efficiency under different carbon conversion rates. The system exergy efficiency increases first and then decreases. With the increase of carbon conversion rate, the energy of coal is more converted into the heat energy of syngas instead of power generation through semi-coke combustion, which reduces the exergy loss. However, the high degree of gasification requires a harsh operating environment, and the input energy increases, which leads to the decrease of system exergy efficiency. The change of syngas composition with carbon conversion rate shown in Fig.3 (b) can also explain the above view. The content of CO increases and the content of H_2 and CO_2 decreases. Table 3 is the exergy efficiency analysis of different gasification agent atmospheres under the conditions of gasification temperature 950 °C, gasification pressure 2MPa, oxygen-coal ratio 0.3 and carbon conversion rate 70 %.



a. The effects of carbon conversion on exergy efficiency.



b. The effects of carbon conversion on syngas component.
Fig.3 The effects of carbon conversion on exergy efficiency and syngas component.

Table 3. System exergy in different gasification atmospheres

Items	H_2O/O_2	CO_2/O_2
Coal input (MW)	0.5774	0.5774
External input (MW)	0.0293	0.0301
Electricity Output (MW)	0.0756	0.0759
Hydrogen Output (MW)	0.2459	0.2595
Exergy efficiency (%)	52.99	55.21

4. Conclusion

(1) With the increase of O_2/Coal and carbon conversion, the exergy efficiency with different gasification agents increases first and then decreases, and there are different values to make the exergy efficiency of different systems reach the highest.

(2) The syngas composition is less affected by O_2/Coal. With the increase of O_2/Coal, CO and CO_2 increase, while H_2 and CH_4 decrease. The carbon conversion rate has a deep influence on the composition of syngas. With the increase of carbon conversion, CO increases and H_2 and CO_2 contents decrease.

(3) Compared with the system using H_2O and O_2 as gasification agents, the system using CO_2 and O_2 as gasification agents has higher exergy efficiency under different oxygen-coal ratios and different carbon conversion rates.

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