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Energy and Carbon Emission Optimisation of Coal to Syngas Process

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Coal gasification to syngas is a common technique for coal utilization and consumes large amount of energy. The design and operation of gasifier, washing column and heat exchangers affect the energy consumption and carbon emission of the whole system. In this work, a coal to syngas process is simulated by Aspen Plus software. Based on the simulation results, the integration among the coal gasification, shift process and rectisol process are analysed; the heat exchanger network (HEN) is optimised to minimize the energy consumption and the carbon dioxide emission. The utility consumption is reduced by 17.4 %, and the emission of CO_2 is reduced by 5.1 %.

1. Introduction

Syngas is an important intermediate product in the application of coal and produced through coal gasification. Its main components are carbon monoxide and hydrogen, and can be used to produce methanol, butanoctanol, ethylene glycol, ammonia, hydrogen, etc. Compared with the direct utilization of coal, coal gasification to syngas is an efficient and more environmentally friendly way to utilize coal, and can improve its utilization value.

In the process of coal to syngas, large amount of energy is consumed. Taking Shanghai Coking Co., Ltd. as an example, the energy consumption of coal-based syngas is 4.216×10^7 kJ/t syngas (Zhang, 2011). In the production process, the main feed stream, coal-water slurry (cold stream) need to be heated, while other process streams (hot streams) require to be cooled. In order to reduce the energy consumption as much as possible, it is necessary to optimise the HEN composed by these hot and cold streams. Along with this, the minimum carbon dioxide emissions can be achieved.

For coal gasification, Wen and Chaung (1979) developed a mathematical model to simulate the Texaco gasifier using coal-water slurries as feed material. Zhang et al. (2014) proposed an Aspen Plus based coal gasification model, in which the gasifier was simulated by two blocks. For the separation of sour gas in the rectisol process, two configurations of single-stage rectisol wash and two-stage configurations are analysed and simulated in Aspen Plus by Sun et al. (2013). Both of them can fulfil the separation requirement, while have different power and other energy demands. Linnhoff and Flower (1978) proposed a two-stage approach to solve the problem of HENs. In the first stage, the preliminary network with the maximum heat recovery is generated. In the second stage, the most satisfactory network is obtained based on the evolution starting from the preliminary network. Tan et al. (2015) evaluated the utilization of energy and carbon emission of a typical Texaco coal gasification process. Pan et al. (2018) built a complex mixed integer nonlinear programming (MINLP) to study the heat transfer intensification in HEN retrofitting; details of exchanger geometry, stream bypassing and splitting, limited minimum temperature difference (LMTD) and its correction, temperature-variation of properties and pressure drops are considered. Jiang et al. (2018) introduced the performance simulation into HEN retrofit model to reassess the performance of reused heat exchange units. Jiang et al. (2020) proposed a multiple objective optimisation model with energy, economic, environmental and engineering quantity indexes considered in the HEN retrofit.

Although many literatures have studied the HEN optimisation of coal gasification process, the three sub-processes are evaluated and optimised independently. There is no report on the evaluation and optimisation with these sub-processes taken as a whole. This work aims to study the integration of three sub-processes of a

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coal to syngas process of China and minimize its energy consumption. Aspen Plus will be used to simulate this process. Then, the minimum energy consumption will be identified according to the simulation results and Pinch Technique. At last, the HENs of three sub-processes are integrated to achieve the minimum energy consumption, as well as the minimum carbon dioxide emission.

2. Simulation of coal to syngas process

Coal to syngas process includes three sub-processes, coal gasification, water-gas shift process and rectisol process. Gasification process has three sections, pretreatment, gasification and grey water treatment. In this process, coal or coal char and gasification agent (air or oxygen) are partially oxidized at high temperature, to convert them into crude gas. Crude gas mainly contains CO, H_2 and H_2O, a small amount of H_2S and COS. It is sent to the Water-Gas Shift Reactor (WGSR) of the water-gas shift unit, where CO reacts with H_2 to generate CO_2. The shifted gas is processed in the rectisol unit to remove impurities, such as CO_2 and H_2S, and obtain the refined syngas. In the process, 5.21×10^8 kg/y coal is processed and 1.47×10^7 Nm^3/y syngas is produced. The main parameters are shown in Table 1. The main flowsheet of this process is shown in Figure 1.

Table 1:Main parameters of coal to syngas process

Parameter	Gasifier	First shift reactor	Second shift reactor	Third shift reactor	CO_2 and H_2S absorber (stage number is 60)	
T (ºC)	1,300	450	280	250	-30	4.5
P (MPa)	6.5	6.15	6.04	5.97	5.45	5.56

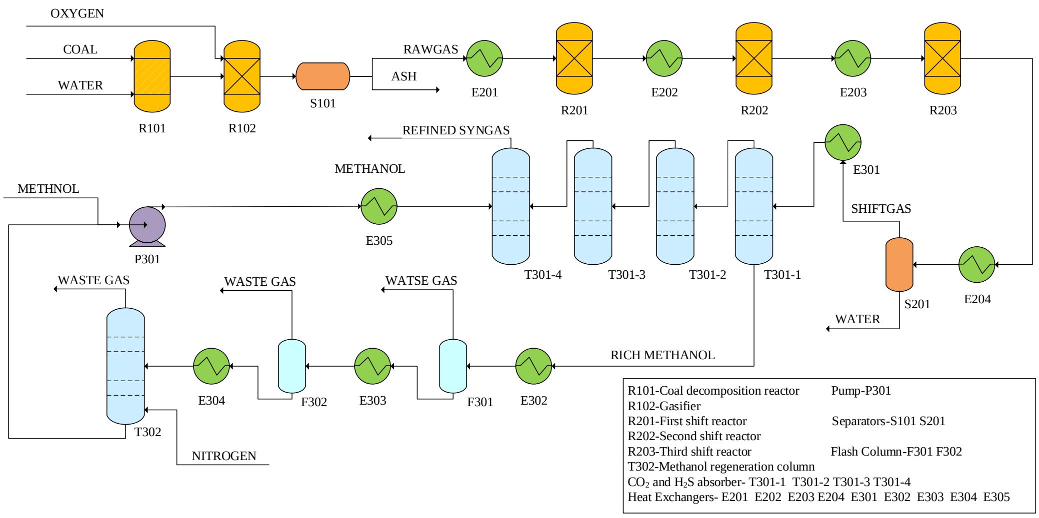

Figure 1: Flowsheet of the coal to syngas process

Based on this flowsheet, the simulation model is built by Aspen Plus 10. In this model, the gasifier is simulated by two reactors, one is RStoic (R101), the other is RGibbs (R102). Rsoic is a stoichiometric coefficient reactor with known reactants and products, and is used to simulate the coal decomposition reaction. The coal is assumed to decompose into elementary substance (C, S, H_2, N_2, O_2 and Cl_2) and ASH in this reactor. These intermediates are sent to the RGibbs reactor, in which the product composition is calculated based on the minimum Gibbs free energy of the reaction equilibrium. In the RGibbs reactor, the main reactions are shown by Eqs(1)-(9).

$$2C+O_2\rightarrow 2CO \quad (1)$$

$$2CO+O_2\rightarrow 2CO_2 \quad (2)$$

$$C+H_2O\rightarrow CO+H_2 \quad (3)$$

$$C+CO_2\rightarrow 2CO \quad (4)$$

$CO+H_2O \rightarrow CO_2+H_2$ (5)

$C+2H_2 \rightarrow CH_4$ (6)

$C+O_2 \rightarrow CO_2$ (7)

$2CO+O_2 \rightarrow 2CO_2$ (8)

$2H_2+O_2 \rightarrow 2H_2O$ (9)

After ash is separated from the gasifier product, the raw gas is obtained and successively sent to the three shift reactors to convert part of CO into CO_2 and H_2 . The aim is to increase the content of H_2 in syngas. The main reaction is shown by Eq(10).

$CO+H_2O \rightarrow CO_2+H_2$ (10)

Since the reaction is a strong exothermic reaction, a lot of heat is produced and can be used to generate steam. The shift gas is sent to the rectisol section, where low-temperature methanol is used as the absorbent to remove the impurities such as CO_2 and H_2S and obtain the refined syngas. Four Rad-Frac blocks are used to simulate the absorber, and are represented by the desulfurization part (T301-1) and decarbonization section (T301-2, T301-3, T301-4).

3. Optimisation of the HEN

3.1 Analysis of HEN

The HEN of current process is shown in Figure 3. The energy is recovered in each sub-process, and there is no heat exchange among three sub-processes. The hot utility consumption (HUC), cold utility consumption (CUC) and CO_2 emission of each sub-process are shown in Table 2. The total HUC is 188,419.6 kW, and the CUC is 149,300.1 kW.

Table 2:Utility consumption and CO_2 emission data

Name	HUC (kW)	CUC (kW)	CO_2 emission (kg/h)	Min. HUC (kW)	Saving potential (%)	Min. CUC (kW)	Saving potential (%)
Gasification	161,848.3	29,972.8	38,381.3	128,466.4	20.62	0	0
Shift	0	89,524.7	0	0	0	89,524.7	0
Rectisol	26,571.3	29,802.6	148,649.1	8,011.3	69.85	11,231.4	62.3
Total	188,419.6	149,300.1	187,030.4	136,477.7	27.57	100,756.1	32.5

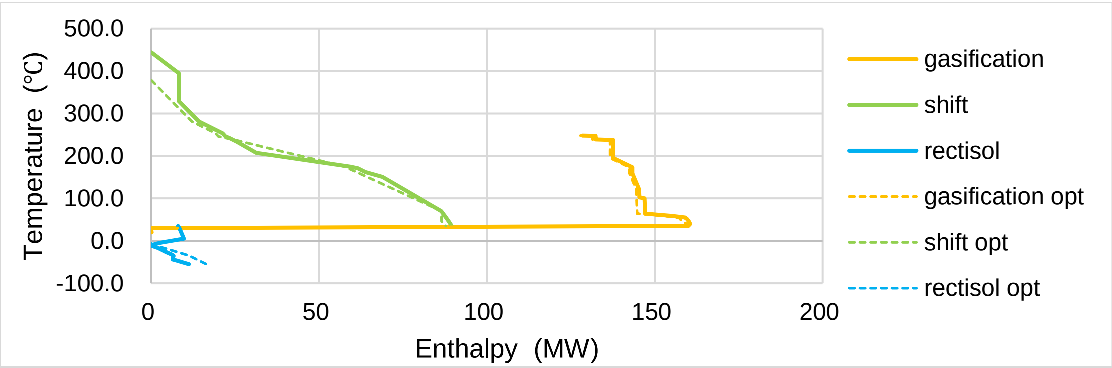

Figure 2: Comparison of Grand Composite Curve before and after optimisation

Based on the simulation data, the Grand Composite Curves (GCC) of three sub-processes are plotted by Aspen Energy Analyzer, as shown in Figure 2. It can be identified that, the minimum HUC of the gasification sub-process is 128,466.4 kW. The minimum CUC for of the shift sub-process is 91,605.8 kW. The minimum HUC and CUC of the rectisol sub-process is 8,011.3 kW and 11,231.4 kW. The detailed data and energy saving potential are shown by Table 2.

It can be seen from Figure 2, there is a large amount of heating demand in the gasification section and cooling demand in the shift section, and the temperature of the former is less than that of the latter. The hot stream of the shift section can be used to provide energy to the cold stream of the gasification section, and the redundant energy can be used to generate steam.

3.2 Optimisation of the HEN

In order to reduce energy consumption, the HEN is optimised based on the Pinch method. The optimal HEN is shown in Figure 4, and the HUC, CUC, GUC and CO_2 emission of each sub-process is shown in Table 3. In Figure 2, the Grand Composite Curve of the HEN after the optimisation is compared with that before the optimisation.

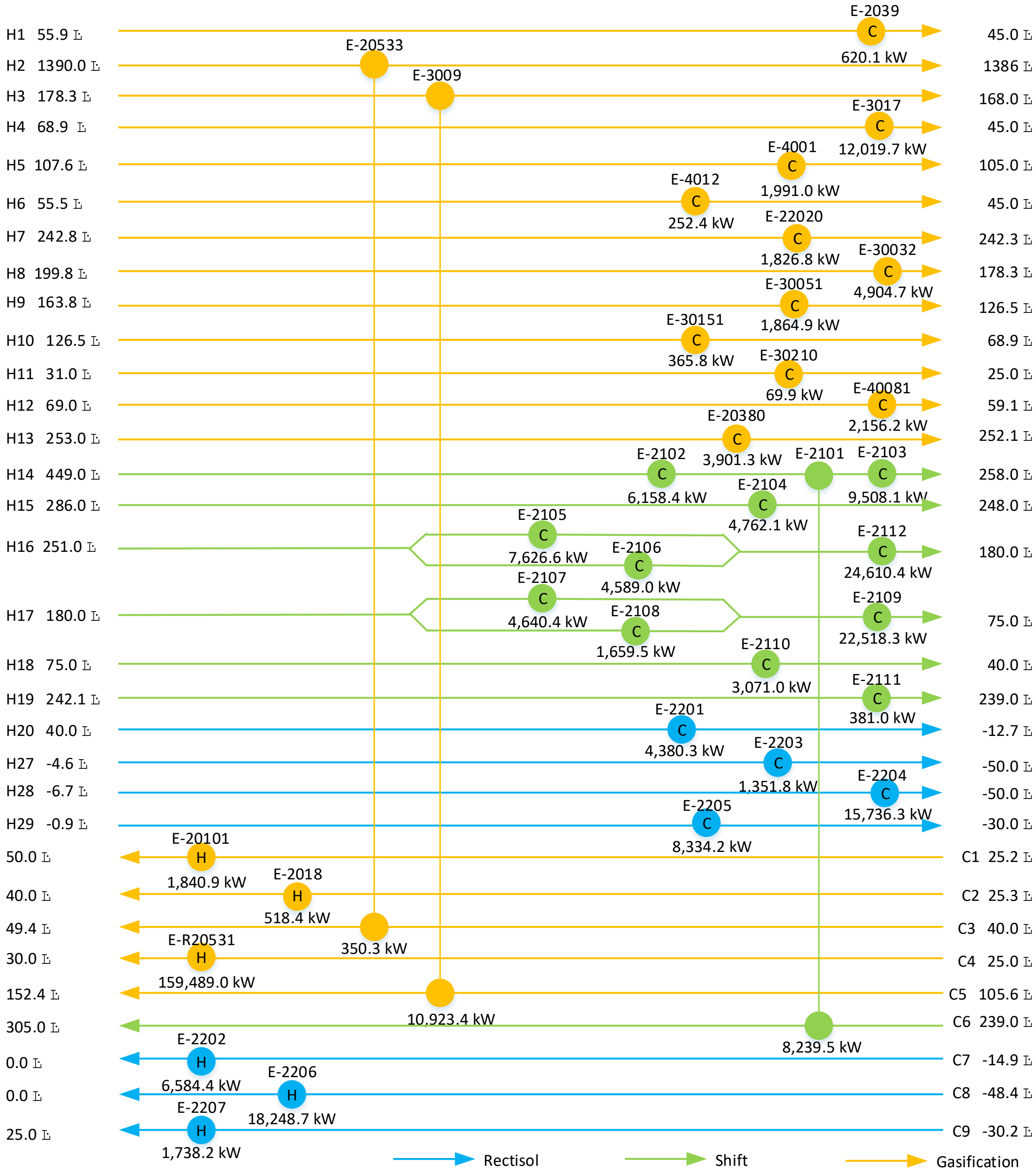

Figure 3: HEN of the current process

Through the comparison, it can be identified that both the HUC of gasification section and shift section are reduced. Although the CUC of the Rectisol section increases, it's heating utility consumption decreases to zero. In the gasification section, there is a large amount of energy demand. However, the corresponding cold stream can only be heated by a furnace and cannot match with other hot streams, as it corresponds the gasification reaction (a strong endothermic reaction) and it is difficult to recover the reaction heat in the furnace. In the optimal HEN, hot streams H4, H11 and H12 are matched with cold streams C7, C8 and C9. Most of the hot streams (H14, H15, H16, H19) in the shift section are used to produce steam (298.1 °C, 0.5 MPa). The total amount of the generated stream is 8.0 × 10^8 kg/y.

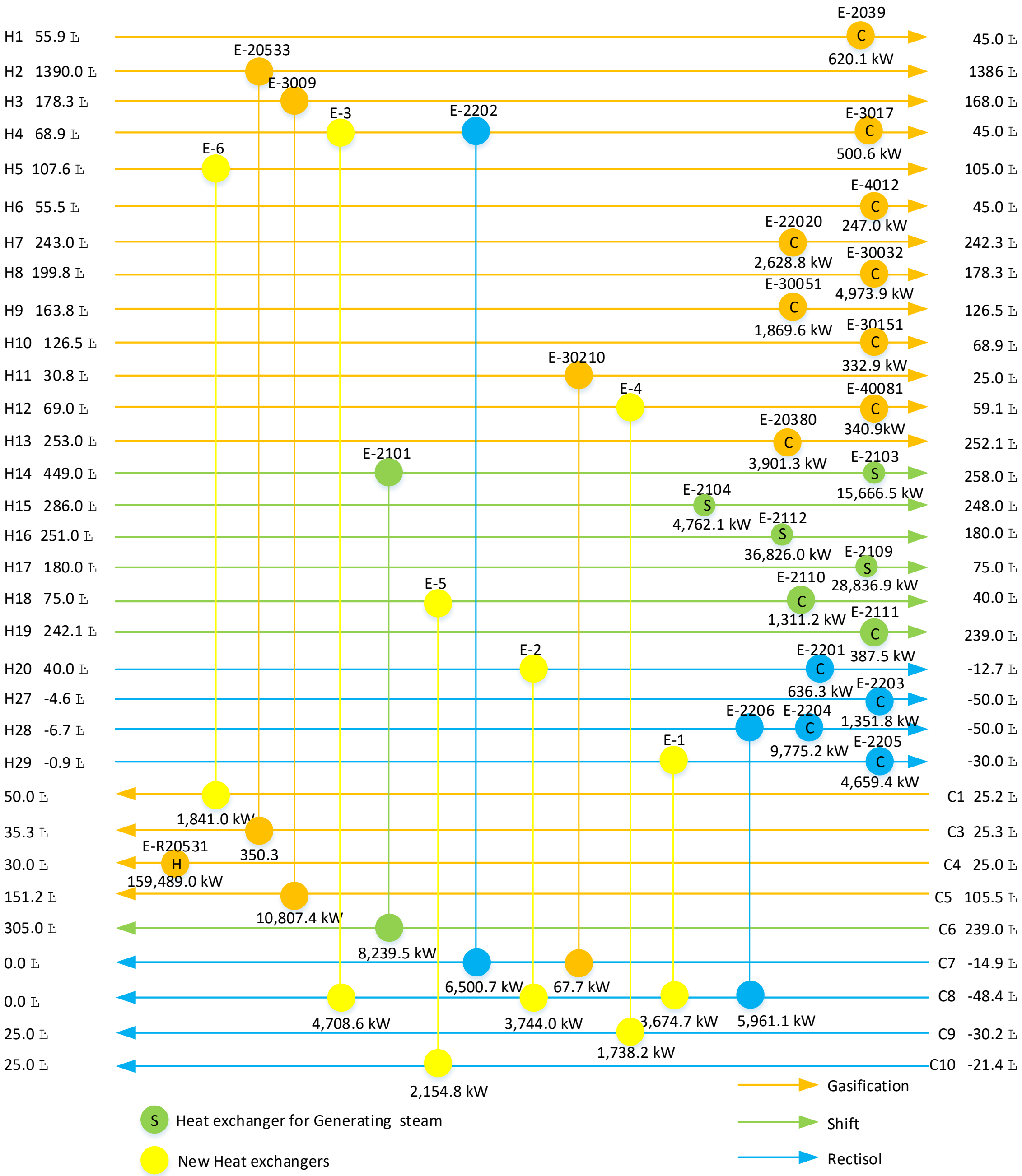

Figure 4: Optimised HEN

Table 3:Utility consumption and CO_2 emission data after optimisation

Section	HUC (kW)	CUC (kW)	GUC (kW)	CO_2 emission (kg/h)
Gasification	159,489.0	15,415.1	174,904.1	37,821.8
Shift	0	87,790.3	87,790.3	0
Rectisol	0	16,422.8	16,422.8	139,625.1
Total	159,489.0	119,628.1	279,117.1	177,473.8

Under the condition of no extra heat exchangers is added, the integration of HEN is carried out among sections. The GUC is reduced by 17.4 %, and the CO_2 emission is reduced by 5.1 %, as shown in Table 4. It can be seen that establishing the heat transfer among different sections is an effective way to reduce the energy consumption.

Table 4: Reduction of utility consumption and CO_2 emission

Name	HUC (%)	CUC (%)	GUC (%)	CO_2 emission (%)
Gasification	1.5	48.6	8.8	1.5
Shift	0	1.9	1.9	0
Rectisol	100	44.9	70.9	6.1
Total	15.4	15.8	17.4	5.1

4. Conclusions

In this paper, the coal to syngas process is simulated and optimised. With the HEN optimised and the heat-exchange among three sections carried out, the utility consumption is reduced by 17.4 % and the emission of CO_2 is reduced by 5.1 %. In this work, only the optimisation of HEN is considered. If the optimisation of shift reactors is considered together with the HEN integration, the energy consumption of the system can be reduced further. This will be studied in the future work.

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