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Life Cycle Assessment of Coal-to-SNG/Methanol Polygeneration Process

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As a kind of clean energy, the demand for natural gas is increasing. However, China's natural gas resources are limited, and their demand growth rate is much higher than the supply. The coal-to-natural gas project alleviates the shortage of natural gas in China by using the abundant coal resources, but it has the problems of single product and poor ability to deal with risks. The coal-to-synthetic natural gas (SNG)/methanol polygeneration process can solve this by coproducing chemicals and have the advantages of high economic benefit and energy saving. The impact of polygeneration process design on carbon emission reduction is still the key issue to be solved urgently. Regarding the coal-to-synthetic natural gas (SNG)/methanol polygeneration process, this paper explores the interaction between polygeneration process design and carbon emissions by using life-cycle assessment method. From the perspective of life cycle, the amount of climate change is evaluated systematically, and the emission factors of each stage are listed. Through sensitivity analysis and Monte Carlo analysis, the breakthrough points of energy saving and carbon emission reduction are found, and the effective carbon emission reduction strategy is also proposed.

1. Introduction

Due to the rapid development of our country's economy, the demand for energy is constantly increasing. China is rich in coal resources, but a large amount of coal use will bring a lot of greenhouse gas emissions, causing pollution to the environment, which runs counter to the goal of achieving carbon peak and carbon neutrality proposed by the Chinese president at the 75th session of the UN General Assembly. Compared with coal, natural gas is cleaner, but Chinese natural gas resources are limited, and the growth rate of natural gas demand is much higher than the supply. Therefore, policies to develop the coal-based synthetic natural gas (SNG) industry have been launched according to the rich coal resources in China. But does this process actually reduce carbon emissions and greenhouse gas emissions? Fu (2010) conducted an inventory analysis on direct and indirect carbon dioxide emissions and greenhouse gas emissions in the whole process of the coal-to-natural gas in different scenarios and found that the coal-to-natural gas in different scenarios and found that the coal-to-natural gas project itself did not play a role in low-carbon emission reduction. Li (2021) studied the application of coal-to-natural gas in different scenarios and found that the coal-to-natural gas project scole and found that the coal-to-natural gas in different scenarios and found that the coal-to-natural gas process could not reduce carbon dioxide emissions but could only achieve emission transfer, that is, high carbon dioxide emissions in the producing area and low emissions in the natural gas use area.

In addition, many scholars optimized the process from the perspective of heat utilization and product diversification. Huang et al. (2018) designed a new coal-based methanol synthesis and power multigeneration process, which significantly reduced the energy consumption of CO₂ capture. Liu et al. (2021) realized energy conservation, emission reduction, and economic benefit improvement of coal-to-natural gas projects by Total Site Heat Integration. Li (2021) simulated and optimized the process of coal-based synthetic natural gas polygeneration methanol process, reducing energy consumption and economic cost. The coal-to-SNG/methanol polygeneration process has strong economic advantages and good prospects. This paper uses the life cycle assessment method to analyze the life cycle carbon emissions and environmental impact of the coal-to-SNG/methanol polygeneration process and analyzes its environmental performance.

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2. Coal-to-SNG/methanol polygeneration process

There are two kinds of coal-to-natural gas technology: one is direct synthesis technology, and the other is indirect synthesis technology. The direct synthesis technology uses one unit to convert coal directly into SNG. It can be divided into the hydrogasification process and the catalytic steam gasification process according to the type of gasification agent (hydrogen or water vapor) when raw coal reacts with the gasification agent.

While the indirect synthesis technology is a "two-step" coal-to-natural gas technology, in which two steps are firstly to convert coal into syngas rich in carbon monoxide and hydrogen, followed by methanation of syngas to obtain SNG. The specific process is shown in Figure 1. The ratio of hydrogen to carbon monoxide in the crude syngas from the coal gasification unit is about 1.45. After adjustment by the cooling conversion unit, the ratio is adjusted to about 3.0. Then entering the low-temperature methanol washing unit to remove acidic gases, such as carbon dioxide and sulfur dioxide, the net syngas obtained can enter the methanation unit to synthesize SNG (Liu et al., 2019).



Figure 1: Coal-to-natural gas process

Methanol is an important intermediate product in the production of aldehydes, acids, ethers, esters, and other chemicals. It can be used in fuel or insecticide and drug processes. It is widely used in China, and the amount of methanol is increasing year by year. At present, the methanol production process mainly consists of coal gasification technology (CGT) using coal as raw material and coking technology (CCT) using coke oven gas (Li et al., 2016). The technical process of coal gasification technology (CGT) is shown in Figure 2.



Figure 2: Coal gasification technology (CGT)



Figure 3: Coal-based synthetic natural gas polygeneration methanol process

As can be seen from Figure 2, the steps before the synthesis of the CGT process are the same as those of coal to natural gas, which provides the possibility for the realization of polygeneration. The optimum ratio of hydrogen to carbon monoxide for methanol synthesis is two, so we only need to adjust the ratio of carbon monoxide and hydrogen in the syngas to realize the simultaneous production of coal to natural gas and methanol. The flow chart is shown in Figure 3.

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3. Introduction to life cycle assessment

Life Cycle Assessment (LCA) refers to the evaluation of the input, output, and potential environmental impact in the life cycle of a product system. It focuses on the whole life cycle of a product, covering the whole process from the acquisition of raw materials needed to produce the product to manufacturing, to use, to disposal after waste. LCA is known as an analysis tool from "cradle" to "grave".

At present, the standard of life cycle assessment is generally recognized as the ISO life cycle assessment standard in the "ISO 14000" series of standards, which stipulates that life cycle assessment consists of four stages, the goal and scope definitions, inventory analysis, impact assessment, and interpretation of results (Guinee et al., 2011), as shown in the figure below.



Figure 4: Life cycle assessment process

In the definition of goal and scope, the reasons for the research, the design parameters to be evaluated, and the scope of the research should be specified. The boundary of the system should also be specified, as well as the selection of functional units. The inventory analysis process follows a series of repeated steps and is an iterative process. It is divided into six parts: preparing data acquisition according to target and scope, data acquisition, data verification, data distribution, data translation to unit process, and data translation to the functional unit. Life Cycle Impact Assessment (LCIA) is the core content of life cycle assessment. Its purpose is to evaluate the impact on the environment based on the inflow and outflow data of the whole life cycle logistics obtained from inventory analysis. The same type of environmental impact is caused by many different environmental impact factors, and one environmental factor can also lead to different environmental impacts. The result and explanation are to summarize and discuss the previous steps, draw a conclusion and propose a plan.

4. Life cycle assessment of the polygeneration process

In this paper, the life cycle assessment software Gabi (version 10.7.0.183) was used to model and analyze the coal-to-SNG/methanol polygeneration process. By investigating the basic data of material and energy inputoutput in each stage of the life cycle of the polygeneration process, Gabi was used to calculate the pollutant discharge list in each stage of the life cycle. Monte Carlo analysis was used to analyze the uncertainty of the input factor and determine the influence of the uncertainty on the results.

4.1 The goal and scope definitions

According to the process of polygeneration technology, the life cycle boundary is divided into the following six parts: coal mining, coal transportation, coal-based synthetic natural gas polygeneration methanol, SNG pipeline transportation, Municipal heating by SNG and methanol use, as shown in Figure 5.



Figure 5: Life cycle boundary of the polygeneration process

The life cycle assessment of the process needs to include the use stage of the product, and SNG and methanol both have more ways of use. It is specified here, among which SNG is used for boiler heating, and methanol is used for bus fuel. The functional unit was defined as input of 1 t lignite / t production.

4.2 Life cycle inventory

The process was analyzed in the inventory based on the literature data (Li, 2021) and the Aspen simulation data. The clean production index of the coal mining stage is selected as level 3 here, in which each 1 t of lignite production requires 0.9 kg of diesel fuel consumption, 28 kWh of electricity consumption, and 0.35 m³ of water consumption. In the coal transportation process, coal is transported from the mining place to the production place, which takes 200 km here. Aspen Plus was used to simulate the synthesis stage of the polygeneration process to obtain the output of natural gas and methanol. The synthetic coal-to-natural gas is transported by pipeline to the place where SNG is used, which is 400 km. The use of SNG is essentially the combustion process of SNG. In this paper, when establishing the life cycle model, only the use of SNG as heating is taken as an example to illustrate, and the thermal efficiency of the SNG heating model is 85 %. The low calorific value of SNG was calculated according to 34.612 MJ/Nm³ (Gong et al., 2015). The methanol obtained is directly used at the production site, so carbon emissions caused by methanol transportation are ignored here. In this paper, methanol obtained from the polygeneration process is used as bus fuel. Methanol fuel can be produced on a large scale with good economy and less conventional pollutants in bus exhaust. The data table is shown below.



Figure 6: Flow diagram of each stock

The above process data is input into the software, and the carbon footprint and environmental impact of the process is analyzed according to the input and output of the process, the amount of electricity used, the amount of heat used, etc., through the database of the software. The process is established as shown in Figure 7.



Figure 7: General flow-chart



Figure 8: Carbon dioxide emission diagram

The emissions in Figure 8 are the carbon dioxide emissions of each stage for each 1 t of coal input, corresponding to total carbon dioxide emissions of 1.19 t. It can be seen from the figure that the carbon emissions are mainly concentrated in the coal-to-natural gas/methanol production stage, coal-to-natural gas heating stage, and methanol use stage, while the carbon emissions of coal transportation and SNG

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transportation stage are relatively small. It can be found that significantly reducing the carbon emissions in the polygeneration process should be started from the three stages by optimizing the process of coal-to-natural gas/methanol synthesis, improving the thermal efficiency of natural gas heating boilers, and reducing the methanol consumption per unit distance of bus travel. The details are listed in Table 1.

	CO ₂	CO	CH ₄
Coal mining (kg/t)	2.100 × 10 ¹	2.128 × 10 ⁻²	1.22
Coal transportation (kg/t· km)	2.370 × 10 ⁻²	4.025 × 10 ⁻⁵	6.117 × 10 ⁻⁵
Polygeneration process (kg/Nm ³)	4.263	4.576 × 10 ⁻³	1.067 × 10 ⁻²
SNG transportation (kg/Nm ^{3.} km)	7.253 × 10 ⁻⁶	9.867 × 10 ⁻⁹	2.023 × 10 ⁻⁸
SNG usage (kg/Nm ³)	1.823 × 10 ⁻¹	4.458 × 10 ⁻³	2.570×10^{-4}
methanol usage (kg/kg)	1.357	1.198 × 10 ⁻²	2.806E × 10 ⁻⁶

4.3 Impact assessment

According to the calculation methods and models proposed by the US National Environmental Protection Agency (EPA) on the influence of global warming, acidification effect, and other twelve influence factors, this paper mainly analyzes the environmental impact of the polygeneration process from the greenhouse effect. According to the regulations of IPCC, the greenhouse-effect causing ability of greenhouse gases is expressed by global warming potential. That is, the equivalent factor of carbon dioxide to global warming is defined as one, and the contribution of other greenhouse gases to global warming is expressed by the carbon dioxide equivalent factor, which means that within a specified period of time (20 y, 100 y, etc.), The greenhouse effect of this gas is equivalent to the mass of carbon dioxide, methane, and carbon monoxide, 25 and 20. The greenhouse effect is shown in the figure below.



Figure 9: Climate change effect diagram of the polygeneration process

4.4 Sensitivity analysis

The parameters of the process and plan were connected, and a sensitivity analysis of parameters was carried out by Gabi. For the main parameters with unknown uncertainty, the variable range of 10 % was allocated to explore the types of parameters that had the greatest influence on the carbon emission of the process. It is found that coal input, methanol and ethylene glycol production, electricity, and steam use have a great impact on climate change, which can be analyzed from the perspective of global energy integration, as shown in Figure 10.



Figure 10: Sensitivity analysis diagram of the polygeneration process

After that, a Monte Carlo analysis was conducted on the process, 10 % of the variable range was allocated, and 10,000 runs were performed. The results show that if the industrial parameters fluctuate by 10 %, the impact on



the environment is mostly concentrated in the range of \pm 6.5 %, and all the fluctuation range is -12.7 % to 19.3 %, indicating that the results were reasonable, as shown in Figure 11.

Figure 11: Monte Carlo analysis diagram of the polygeneration process

5. Conclusions

In this paper, the life cycle evaluation method is used to investigate the input and output, greenhouse gas emissions, and environmental performance of the coal-to-SNG/methanol polygeneration process. It is found that 83.4 t of coal-to-natural gas and 117 t of methanol can be produced when 645 t of lignite is imported. In terms of greenhouse gases, 1.19 t of carbon dioxide output corresponds to unit input. The carbon emissions and climate change effect are mainly concentrated in the coal-to-natural gas/methanol production stage, coal-to-natural gas heating stage, and methanol use stage, while the carbon emissions of coal transportation and SNG transportation stage are relatively small. Through sensitivity analysis, it can be found that coal input, methanol and SNG production, electricity, and steam use have a great impact on climate change, and the subsequent analysis should start from the Total Site Heat Integration. Monte Carlo analysis of the process found that if a 10 % fluctuation occurred in the industry, the environmental impact fluctuated in the range of -12.7 % to 19.3 %, most concentrated in ± 6.5 %, which is acceptable. So far, we have obtained the carbon emission and environmental impact of the coal-to-SNG/methanol polygeneration process, which can provide environmental data support for the subsequent development of the co-production process.

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