Process route and economic analysis of hydrogen production from oil shale

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Abstract. The development of hydrogen production process can provide a new way to use oil shale with high value and low carbon emission. However, the current research only considers hydrogen as a small amount of by-product during oil shale processing, and there is a lack of understanding of the technology aimed at hydrogen production. The technical route of hydrogen produced from oil shale is proposed in this study. The complete process from oil shale raw material to hydrogen product is designed, including six modules of pyrolysis, combustion, gasification, reforming, purification, and flue gas treatment. The effects of key operating parameters on oil shale transformation, product composition, and energy consumption characteristics are analyzed. The results show that the proposed route in this study can produce industrial hydrogen with 99% purity. Under the condition that the CO_2 removal rate is 90% and the exhaust gas meets the emission standard, the efficiency of hydrogen production from oil shale is 6.26 Nm^3-H_2/t-shale, with a system energy efficiency of 75.61% and an exergy efficiency of 46.43%. Economic analysis shows that the annual profit and return on investment of this process are significantly higher than that of other shale refining processes. This research provides technology options for hydrogen production and the high-value, clean, and low-carbon utilization of oil shale.

Keywords: Hydrogen production; Oil shale; Carbon emission reduction; Economical analysis

1 Introduction

In recent years, the energy demand has further increased with the rapid economic development of various countries. Due to limited reserves, conventional fossil energy is tight[1]. As an unconventional fossil fuel with abundant reserves and wide distribution, oil shale is considered one of the alternatives to traditional fossil fuels[2]. Oil shale is a sedimentary rock containing solid organic matter (kerogen). Kerogen, as a macromolecular compound with a complex structure, is insoluble in conventional organic solvents[3]. At present, many countries have begun to study more efficient, environmentally friendly, and economical oil shale deep processing technology.

The shale oil produced by oil shale pyrolysis contains many impurities, especially unsaturated hydrocarbons, sulfur and nitrogen. Shale oil hydrogenation is expected to

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be an effective way to solve this problem[4-8]. According to the Global Investment Council[9-10], the average cost of extracting shale oil is $40 to $60 per barrel. With the recent decline in crude oil prices, shale oil is trading at a discount to crude oil. As a recognized clean energy, hydrogen energy is regarded as the main terminal energy form in the future.

The concept of hydrogen production from shale oil focused on the minimum energy consumption is proposed in this paper. The pyrolysis of shale oil and gas is used to produce hydrogen, while the waste shale generated by pyrolysis is used to burn and supply energy, solving the problem of heat source for the whole system. A model for technical & economic analysis and exergy efficiency analysis was built.

1.1 Design regulation

In this paper, oil shale is modeled as three sub-flows of moisture, kerogen and minerals. New Albany oil shale was used in the simulation with a capacity of 225 $t{\cdot}h^{-1}$. The Redlich-Kwong-Soave (RK-SOAVE) equation is chosen as the physical property method for oil shale pyrolysis. The specific composition and elemental analysis results of oil shale are shown in Table 1.

Table 1. Composition and element analysis of oil shale

	Component（%）			Elemental Analysis（wt. %）				
	Moisture	Kerogen	Minerals	C	H	O	N	S
Oil Shale	3.00	15.23	81.77	78.33	8.93	6.37	2.56	3.81

The process is assumed to be steady-state. The oil parent material is retorted to produce shale oil, retorted gas and waste shale, while the mineral matter is inert. To simplify the simulation process, only the following products are considered in the simulation: H_2, CO, CO_2, CH_4, H_2O, H_2S, NH_3, C_2H_6, C_3H_8, C_4H_{10}, Oil, Char, SO_2, NO. Oil is composed of $C_{12}H_{24}$. The chemical reaction is regarded as the ideal process, and the pressure loss of the whole process is not considered.

1.2 Hydrogen production system model

To simulate the hydrogen production process by Aspen Plus, the whole process is divided into six subsystems: pyrolysis, combustion, gasification, reforming, carbon capture, and flue gas treatment. The system stream is shown in Fig. 1.

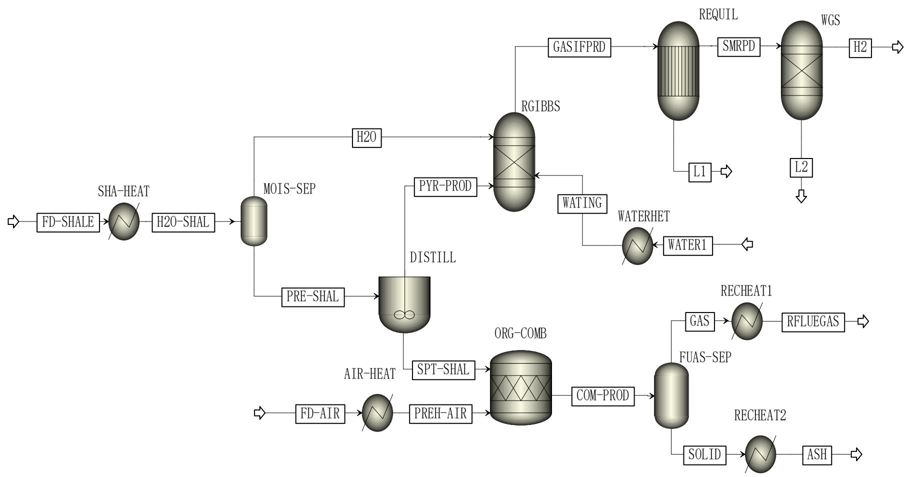

Fig. 1. General stream of oil shale hydrogen production system

1.3 Assessment indicator system

The energy balance of the system is calculated according to Equation (1), Where Q represents the input heat of the system, W represents the income work, H_n represents the enthalpy value of the logistics, and Q_{loss} refers to the heat loss of the system.

$$Q+W+\sum H_{n,\text{in}}=Q_{\text{loss}}+\sum H_{n,\text{out}} \tag{1}$$

The energy consumption (E_x) of the entire process system is composed of electricity and another indirect working medium energy supply, as shown in Equations (2) and (3):

$$E_x = x_{\text{oil}} m_{\text{oil}} \tag{2}$$

$$m_{\text{oil}} = \sum_i y_i m_i \tag{3}$$

where x_{oil} is the conversion coefficient between standard oil and standard electricity, moil is the standard fuel consumption, y_i is the conversion coefficient between other indirect working medium and standard oil, and mi is the quality of another indirect working medium.

The exergy balance of the system is shown in Equation (4), where E represents exergy flowrate. Exergy includes exergy value ΣE_{in} of input logistics, exergy value includes ΣE_{out} of output logistics, and exergy loss Ii of unit equipment. The enthalpy of matter, work, and heat as well as the exergy calculation methods refer to the new national standard[11].

$$\sum E_{\text{in}} = \sum E_{\text{out}} + \sum I_i \tag{4}$$

Exergy analysis mainly evaluates the thermodynamic performance of a system by exergy efficiency. Based on the exergy balance of the system, the numerical value of the process or thermodynamics is described. Exergy efficiency is defined as the ratio of exergy output to exergy input, or exergy income to exergy payment, as shown in Equation (5).

$$\eta = E_{\text{out}} / E_{\text{in}} \times 100\% \tag{5}$$

Total investment expense (TCL) mainly includes fixed asset investment and working capital, which can be calculated by Equation (6).

$$TCL = I_{EI} + I_{IPE} + I_{BL} + I_{ES} + I_{CCF} + I_{WCC} \tag{6}$$

where I_{EI} is equipment and installation costs, I_{IPE} is instrumentation, piping and electrical costs, I_{BL} is building and land costs, I_{ES} is engineering and supervision costs, I_{CCF} is construction and contractor fee costs, and I_{WCC} is working capital and contingency costs.

Total cost of production (TPC) mainly includes manufacturing costs and general expenses, which can be calculated by Equation (7).

$$TPC = C_{\text{R}} + C_{\text{U}} + C_{\text{OM}} + C_{\text{FC}} + C_{\text{POC}} + C_{\text{GE}} \tag{7}$$

where C_R is the cost of raw materials, C_U is the cost of utilities, C_{OM} is the cost of operation and maintenance, C_{FC} is the fixed costs (including depreciation costs, local taxes, insurance and rent), C_{POC} management costs, C_{GE} is the distribution and selling cost (including administrative, sales, research & development and finance expenses). ROI refers to the ratio of the total annual profit in a normal year after the project reaches the design capability or the ratio of the average annual total profit in the production period to the total project investment, and is defined as Equation (8).

$$ROI = \frac{ASR - APC}{TCL} \times 100\% \tag{8}$$

2 Results analysis

2.1 Simulated result

The material simulation results of system input and output are shown in Table 2. In the output substances, the most is the purified flue gas followed by ash, and the least is dilute HNO_3. The energy consumption of the oil shale hydrogen production process includes heating heat source, compressor work, and cooling water condensation. To facilitate statistics, according to the standard[12], the energy consumption of each energy consumption module is converted into electricity consumption, and the total energy consumption of the whole system is 43.40 MW.

Table 2. Simulation results of shale-to-hydrogen process

Input	Mass flowrate ($kg\cdot h^{-1}$)	Output	Mass flowrate ($kg\cdot h^{-1}$)
Oil shale	225000	H_2	7247
Air	219770	Ash	183983
Water	179212	Flue gas	175021
		SO_2	12115
		CO_2	83145
		HNO_3	4838
		Waste water	157633
Total	623982		623982

2.2 Thermomechanical analysis

Energy and exergy balance are carried out according to 2.4 technical guidelines and Chemical properties handbook-enthalpy[13]. The results of the system energy balance are listed in Table 3. The energy output of hydrogen is relatively large, followed by heat loss, and the lowest is dilute HNO_3. The energy efficiency of the whole system is 76.25%, and the heat loss ratio is about 23.75%. The main loss comes from the heat dissipation in the process of hydrogen purification and flue gas treatment.

Exergy data are listed in Table 4 according to the calculation method of the new national standard Exergy value. Exergy loss in the system mainly includes exergy loss caused by heat dissipation from high-temperature fluid to the outside and exergy loss caused by heat dissipation during heating.

Table 3. Energy balance in the system

Input	Energy flowrate (kJ·h-1)	Output	Energy flowrate (kJ·h-1)
Oil shale	1.67×109	H2	8.18×108
Air	4.51×108	Ash	3.37×108
Water	2.07×108	Flue gas	2.88×108
		SO2	4.05×107
		CO2	1.67×108
Electrical power	1.20×108	HNO3	9.77×106
		Waste water	1.89×108
		Energy loss	5.96×108
Total	2.44×109		2.44×109

Table 4. Exergy balance in the system

Input	Exergy flowrate ($kJ\cdot h^{-1}$)	Output	Exergy flowrate ($kJ\cdot h^{-1}$)
Oil shale	1.60×10^9	H_2	5.28×10^8
Air	1.93×10^5	Ash	3.92×10^7
Electrical power	1.20×10^8	Heat	1.70×10^8
		Flue gas	5.11×10^6

		SO_2	1.41×10^7
		CO_2	4.32×10^7
		HNO_3	1.48×10^4
		Waste water	1.05×10^6
		Exergy loss	9.24×10^8
Total	1.72×10^9		1.72×10^9

As shown in Table 4, the highest input exergy is oil shale, followed by compressor work, accounting for 6.95% of the total exergy, the least is the water with normal temperature, the exergy value of exergy is 0. Output exergy accounts for the largest proportion of exergy loss, while exergy value of hydrogen is the second highest, and that of dilute HNO_3 is the lowest.

2.3 Economical Analysis

According to the start-up time of 8,000 hours a year, the oil shale processing capacity is 225 t/h. The equipment investment for the hydrogen production process of oil shale is calculated according to the technical evaluation indexes in Section 2.3. The estimation model is based on reference[14], the total investment cost of equipment for the hydrogen production process and refining process of oil shale reported in reference[15] is calculated by Equation (6), and the results are 1.489 billion CNY and 1.114 billion CNY respectively, as shown in Fig. 2a. The total investment cost of the oil shale hydrogen production process is 375 million CNY higher than that of the existing oil shale refining process. The main reason is that the shale hydrogen production process increases the methane steam reforming and flue gas treatment process compared with the existing process, which makes the equipment cost and pipeline cost increase correspondingly in the direct costs. Regarding the indirect cost, only engineering design costs increase accordingly.

Production cost is the most important factor to determine the economic efficiency of the manufacturer. Combined with the research data[14] and Equation (7), the total production cost of the hydrogen production process of oil shale and the existing oil shale refining process is finally obtained as 865 million CNY and 626 million CNY, and the results are shown in Fig. 2b. The total investment cost of the hydrogen production process of oil shale is 239 million CNY higher than that of the existing oil shale refining process[15]. In the process of producing hydrogen from oil shale, hydropower consumption is higher, and hydropower consumption is in the process of reforming, hydrogen purification, and flue gas treatment.

Assume that the construction period of the project is one year and the production period is 25 years. According to the financial model of the industrial economic model, it is calculated that the gross income of the hydrogen production process of oil shale is 1.333 billion CNY/year, the total profit is 469 million CNY/year, and the corporate income tax is 25%, the net profit is 352 million CNY/year. Compared with the existing oil shale refining process, the total profit increased by 202 million CNY/year, and the net profit increased by 141 million CNY/year. According to formula (8), the investment profit rate of the hydrogen production process of oil shale and the existing Fushun shale refining process is 23.60% and 18.89%, there is an increase of 4.71 percentage points, as shown in Fig. 2c. Therefore, hydrogen production from oil shale can significantly improve the economic benefits of oil shale development and utilization.

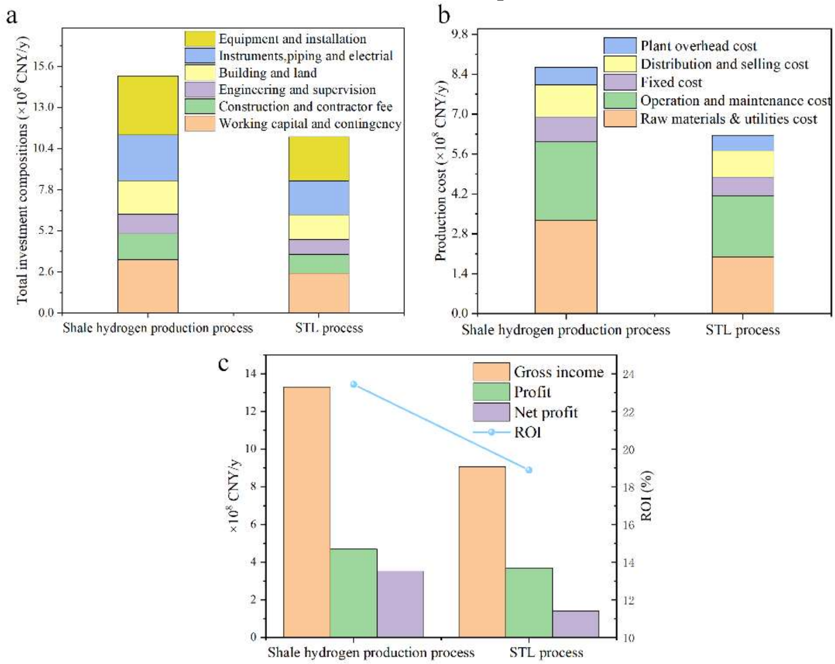

Fig. 2. Economic comparison between hydrogen production from oil shale and existing STL process.

a- Total investment compositions of shale hydrogen production process and STL process.

b- Production cost compositions of hydrogen production process and STL process.

c- Gross income and ROI of shale hydrogen production process and STL process.

3 Conclusion

In this work, a new hydrogen production process of oil shale is designed and studied from the point of thermodynamics and economy of hydrogen production. The following conclusions are obtained.

The idea of hydrogen production from oil shale with high yield is put forward, and the process system configuration is established. In the final product, the H_2 output is 7247 $kg \cdot h^{-1}$, the purity is 99%, the system energy efficiency is 75.61%, and the system exergy efficiency is 46.43%.

The designed oil shale refining process produces hydrogen by gasification of the generated dry distillation oil and gas, and then by purification to obtain high-purity hydrogen and CO_2. Compared with the existing oil shale refining process, the economic benefit has been significantly improved, the total investment cost of the new process is

1.489 billion CNY, the total production cost is 865 million CNY/year, the gross annual income is 1.333 billion CNY, the profit is 469 million CNY/year, the net profit is 352 million CNY/year, and the investment profit rate is 23.60%.

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