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Innovative Coal-to-Olefin Process Integrated with Sustainable Renewable Electricity and Green Hydrogen

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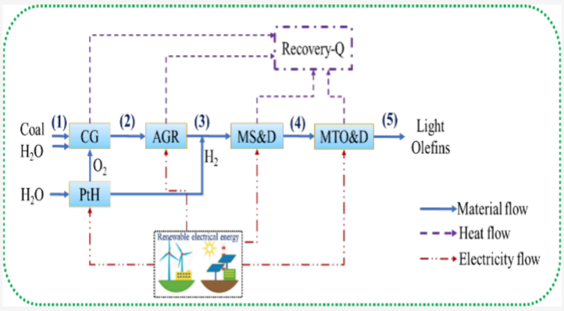
ABSTRACT: The conventional Coal-to-Olefins (CTO) process is plagued by high CO_2 emissions and significant water consumption. To address these issues, two routes are designed and modeled to compare with the conventional CTO route in terms of energy consumption, CO_2 emissions, water consumption, and economic performance: the Renewable Electricity coupled to CTO process (RE-CTO) route and the Renewable Electricity and Green Hydrogen coupled to conventional CTO route (RE-GH-CTO). Introducing renewable electricity into the CTO process enhances the energy efficiency, reduces grid loads, and decreases indirect CO_2 emissions. The integration of green hydrogen technology removes the air separation unit and water−gas shift unit, shortens the process, reduces energy consumption, and improves CO_2 utilization. The RE-GH-CTO route can motivate a multienergy integration and complementation, improve energy efficiency, and boost light olefins productivity. The results showed that the RE-GH-CTO route improved energy efficiency and carbon utilization efficiency by 14.51% and 40.80%, and reduced carbon dioxide emissions and water consumption by 76.71% and 32.68% compared with the conventional CTO process. In addition, the production cost of the RE-GH-CTO route is 8.30% lower than the conventional CTO route. This innovative route provides a promising approach for introducing green hydrogen for CO_2 utilization and the sustainable conversion of coal to chemicals.



1. INTRODUCTION

Light olefins are key chemical feedstocks that play an irreplaceable role in modern life. In 2023, China has surpassed the United States to become the largest producer and consumer of olefins in the world.[1] Ethylene consumption in China has grown from 14.97 million tons in 2010 to 33.87 million tons in 2023, which is expected to reach 86.4 million tons by 2030.[2] The key raw materials for producing olefins are crude oil, natural gas, coal, and biomass.[3,4] In China, the energy structure is characterized by an abundance of coal, scarcity of oil, and limited natural gas resources.[5] Thus, Coal-to-Olefins (CTO) has become a crucial alternative method for olefin production in China. Moreover, it is well-known that the service life of crude oil and natural gas resources is limited to 40−60 years, whereas coal availability is estimated at around 230 years.[6] Once oil and gas run out, the clean and efficient use of coal will need to be reconsidered. In this context, there has been a resurgence of interest in coal conversion technologies for chemical production. The flow diagram of the conventional CTO route is illustrated in Figure 1. This process consists of six key units: air separation unit (ASU), coal gasification (CG), water−gas shift (WGS), acid gas removal (AGR), methanol synthesis and distillation (MS&D), methanol to olefins and distillation (MTO&D).

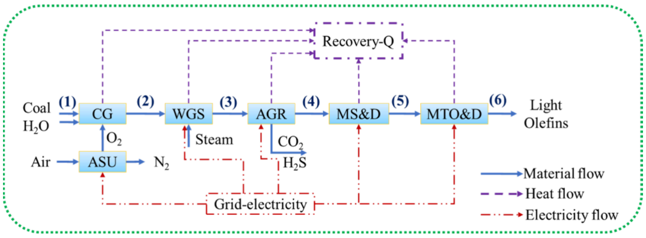


Figure 1. Schematic diagram of the conventional CTO route.

The conventional CTO route faces significant challenges in high energy consumption and substantial CO_2 emissions, with the high energy consumption primarily occurring in ASU and CG units and the high CO_2 emissions originating from the WGS and AGR units.[7] Alarmingly, the CO_2 emission intensity of the CTO route ranges from 7.1 to 10 tons of CO_2/t olefin.[8] Research indicates that the heavy reliance on coal results in

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significant CO_2 emissions, with carbon utilization efficiency falling below 50%.[9]

Under the carbon peak and neutrality targets, it is essential to integrate hydrogen-rich resources into conventional coal-based processes and reduce CO_2 emissions in the coal-based chemical industry. For instance, Xiang et al. enhanced conventional CTM processes with chemical looping hydrogen and air separation, boosting carbon utilization from 38.4% to 56.1% and cutting CO_2 emissions from 1.47 to 0.71 kmol/kmol methanol.[10] This advancement represents a significant step toward a more sustainable future in the chemical industry. Huang et al. created a methanol poly generation process that cuts CO_2 capture energy use to 0.7 GJ/t-CO_2, achieving a 40.6% reduction compared to traditional coal-to-methanol methods.[11] Qin et al. created a hybrid energy system to tackle the low hydrogen content in coal. Their innovative design shows that adding hydrogen from biomass cogasification and solar can improve carbon utilization (from 39.41% to 41.49%). However, it may reduce the energy efficiency and economic performance. This highlights that integrating renewables with fossil fuels is not always advantageous for chemical production.[12] Qian et al. have developed a new process that combines CG with coke-oven gas trireforming to produce methanol. This innovative approach boosts carbon utilization by 25% and energy efficiency by 10%, while cutting CO_2 emissions by 44%, compared to traditional methods.[13]

In recent years, the rapid expansion of renewable energy and power-to-hydrogen (PtH) technology has significantly accelerated the advancement of green hydrogen solutions.[14] Moreover, electrolytic hydrogen is considered to integrate with the conventional coal chemical industry.[15] Wang et al. introduced a groundbreaking process for methanol production using pulverized coal gasification and green hydrogen, achieving near-zero carbon emissions. CO_2 emissions dropped from 1.9 to just 0.035 t CO_2/t MeOH. Compared to traditional methods, this innovation boasts 88.87% lower CO_2 intensity, 130.77% higher carbon utilization, and 39.64% greater energy efficiency.[16] However, the water consumption in the CG unit and PtH process is significantly higher. China's major coal reserves are located in Shanxi, Shaanxi, Inner Mongolia, Ningxia, and Xinjiang, regions that are generally water-scarce. But the conventional coal chemical industry requires a large amount of water resources in the CG unit for producing crude syngas and WGS[17] unit to adjust the H/C ratio. The water consumption is 26−30 t/t olefins in the conventional CTO process.[18] A comparative analysis of energy and water use, along with CO_2 emissions, is crucial for driving energy conservation and reducing emissions in the olefins industry.

To address the challenges of high energy and water consumption as well as elevated carbon dioxide emissions, numerous experts and scholars have conducted extensive research. While we have made strides in reducing CO_2 emissions and improving energy efficiency, the issue of excessive water consumption persists. Our goal is to develop a pathway that achieves low CO_2 emissions, reduce the intensity of water consumption, improve energy efficiency, and enhance production yields.

Exploring the feasibility of low CO_2 emissions in the CTO route. This study proposes integrating renewable electricity with a CTO (RE-CTO) and combining it with green hydrogen production (RE-GH-CTO). The advantages of the RE-GH-CTO route are as follows:

(a) This process eliminates the need for ASU, significantly reducing energy consumption. The oxygen required for CG is sourced from the PtH process.
(b) By avoiding the WGS unit, the process minimizes CO_2 production, contributing to a lower carbon footprint.
(c) The crude syngas generated from CG undergoes a simplified AGR process, achieving nearly 100% separation of H_2S without the need for CO_2 purification. The produced CO, CO_2, and renewable hydrogen are subsequently utilized in the MS unit.
(d) Coal gasification coupled with green hydrogen production has the advantage of near-net CO_2 emission and adjustable H_2/CO ratio in a range of 1.0−2.0, which results in a high carbon utilization efficiency.
(e) Low water consumption and high yield of light olefin.
(f) Achieves multienergy integration and complementarity and improves the energy efficiency.

Our literature review reveals a gap: no articles focus on the operational parameters of CTO, RE-CTO, and RE-GH-CTO routes. We have developed a comprehensive steady-state model to evaluate the technical, economic, and environmental performance. This analysis includes a comparison of carbon utilization efficiency, energy efficiency, CO_2 emissions, water usage, and production costs.

2. MODELING AND OPTIMIZATION

In this study, we based our coal-to-olefin scale on the Shenhua project, which produces 0.6 Mt/y of light olefins using raw coal, about 2.28 Mt/y. With an annual production period of 8000 h, this results in a steady output of 0.6 Mt/y.

The conventional CTO route involves eight key units, as illustrated in Figure 1. Initially, pulverized coal reacts with oxygen from the ASU and undergoes gasification to produce crude syngas in the CG unit. To meet the hydrogen-to-carbon (H/C) ratio requirements for methanol synthesis, a portion of the crude syngas is directed to the WGS unit to generate additional hydrogen. The crude syngas is transported to the AGR unit, where CO_2 and H_2S are effectively removed. The resulting purified syngas is then utilized for methanol synthesis, contributing to sustainable energy solutions.

The RE-CTO route is proposed and demonstrated in Figure 2. Compared with traditional CTO route, all electricity in the grid is replaced by renewable electricity in the RE-CTO route. Especially, the electricity for transmission equipment comes from solar or wind power.

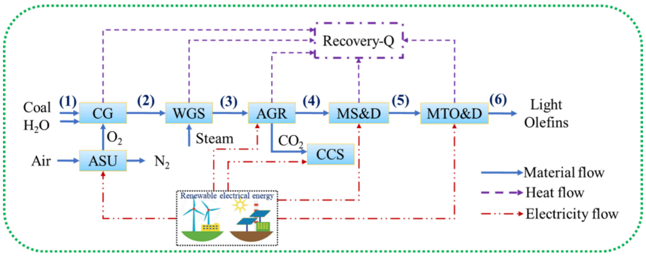

Figure 2. Schematic diagram of the RE-CTO route.

The RE-GH-CTO route has been introduced, as illustrated in Figure 3. This innovative approach begins with pulverized coal reacting with oxygen in the PtH unit to produce crude syngas within the CG unit. Notably, this crude syngas can be directly sent to the AGR unit for H_2S removal, bypassing the

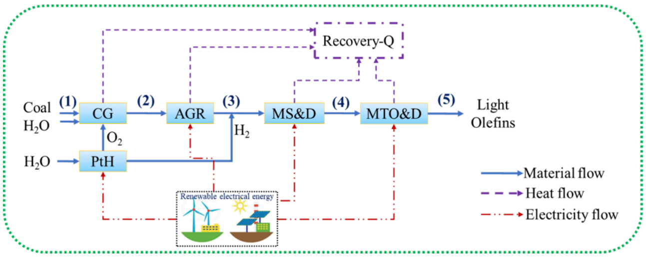

Figure 3. Schematic diagram of the RE-GH-CTO route.

need for a WGS unit. Additionally, GH generated from the PtH unit plays a crucial role in adjusting the H/C ratio. The resulting mixture of CO, CO_2, and H_2 is then processed in the MS unit to produce methanol. The methanol enters the MTO unit, and crude olefins are separated by the "front-end depropanization" process. Renewable electricity and green hydrogen production were integrated with the CTO process.

The raw coal can be examined, and its properties are detailed in Table 1. Utilizing Aspen Plus (Version 11.0), we identified the coal components as being unconventional. For our analysis, we employed the HCOALGEN model to assess enthalpy and the DCCOALIGN model for density evaluation.[19]

Table 1. Analysis Results of the Raw Coal

ultimate analysis (wt%)		proximate analysis (wt%)	
carbon	73.64	moisture content	5.81
hydrogen	5.24	fixed carbon	52.93
nitrogen	1.13	volatile matter	39.54
sulfur	2.63	ash	7.53
oxygen	9.83		

2.1. CTO Route. *2.1.1. Coal Gasification Unit.* In this work, CO_2 was used as the coal carrier instead of N_2 to reduce the number of diluents in syngas, as shown in Figure 4. The gasifier operates at a high temperature of approximately 1554 °C, where coal, steam, oxygen, and CO_2 are introduced. One of the key innovations is the recovery of heat from crude syngas, which is then used to produce high-pressure steam (HPS) for power generation via steam turbines. For modeling the coal gasification process, the pyrolysis approach is used the RYield block to effectively decompose coal into various components,[20−23] including CH_4, C_2H_6, CO, CO_2, C_6H_6, H_2, H_2O, N_2, H_2S, and char, as outlined in eq 1.

$$\begin{aligned}\text{coal} \rightarrow\ & \text{char} + H_2 + CH_4 + C_2H_6 + CO + CO_2 \\ & + C_6H_6 + H_2O + N_2 + H_2S\end{aligned} \tag{1}$$

$$\begin{aligned}& C + \frac{1}{n}O_2 \rightarrow \left(2 - \frac{2}{n}\right)CO + \left(\frac{2}{n} - 1\right)CO_2 \\ & \quad \Delta H_{298.15K} = -110.5\ \text{kJ/mol}\end{aligned} \tag{2}$$

$$C + CO_2 \rightarrow 2CO \qquad \Delta H_{298.15K} = +172.5\ \text{kJ/mol} \tag{3}$$

$$C + H_2O \rightarrow CO + H_2 \qquad \Delta H_{298.15K} = +131.3\ \text{kJ/mol} \tag{4}$$

$$C + 2H_2 \rightarrow CH_4 \qquad \Delta H_{298.15K} = -74.6\ \text{kJ/mol} \tag{5}$$

$$H_2 + 0.5O_2 \rightarrow H_2O \qquad \Delta H_{298.15K} = -242\ \text{kJ/mol} \tag{6}$$

$$\begin{aligned}& CH_4 + 0.5O_2 \rightarrow CO + 2H_2 \\ & \quad \Delta H_{298.15K} = -35.5\ \text{kJ/mol}\end{aligned} \tag{7}$$

$$CO + 0.5O_2 \rightarrow CO_2 \qquad \Delta H_{298.15K} = -283.1\ \text{kJ/mol} \tag{8}$$

$$\begin{aligned}& C_2H_6 + O_2 \rightarrow 2CO + 3H_2 \\ & \quad \Delta H_{298.15K} = -120.6\ \text{kJ/mol}\end{aligned} \tag{9}$$

$$\begin{aligned}& C_6H_6 + 3O_2 \rightarrow 6CO + 3H_2 \\ & \quad \Delta H_{298.15K} = -124.3\ \text{kJ/mol}\end{aligned} \tag{10}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \qquad \Delta H_{298.15K} = -41.2\ \text{kJ/mol} \tag{11}$$

$$\begin{aligned}& CH_4 + H_2O \rightarrow CO + 3H_2 \\ & \quad \Delta H_{298.15K} = +205.9\ \text{kJ/mol}\end{aligned} \tag{12}$$

In the coal pyrolysis process, the interaction of volatile matter and char with oxygen and steam initiates key reactions, as detailed in eqs 1−12. To effectively simulate the gasification and combustion stages, the RGibbs block can be utilized, which is based on Gibbs free-energy minimization.[24−26]

2.1.2. WGS Unit. WGS unit adjusts the H/C ratio for methanol production using a low-temp shift reactor at 250 °C and 2.5 MPa. This process can be summarized by the equations provided in eq 11. Crude syngas heat is recovered via a waste heat boiler before entering WGS,[27,28] where CO and H_2O convert to H_2 and CO_2, as shown in Figure 5. The processed syngas achieves an H/C ratio of 2.15.

2.1.3. AGR Unit. The Rectisol process is a widely recognized method for efficiently removing H_2S and CO_2 in large-scale CTM operations.[29] This advanced process includes key components such as the acid gas absorber, CO_2 desorber, H_2S concentrator, and regenerator sections, ensuring optimal performance and reliability in gas treatment.

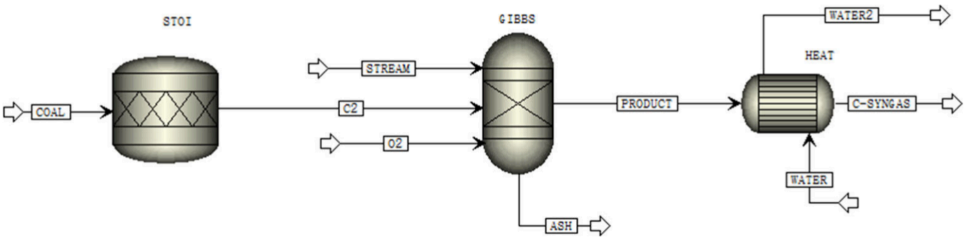

Figure 4. Process flowsheet of the coal gasification unit.

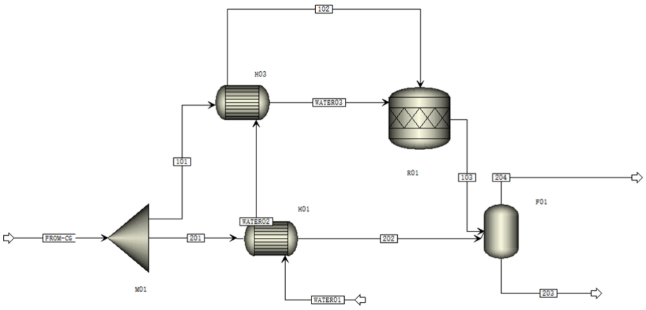

Figure 5. Process flowsheet of the WGS unit.

The syngas was introduced into the scrubber (T0101, T0102, T0103) mixed with the methanol release gas as shown in Figure 6. Methanol was used as the solvent. H_2S and CO_2 were removed, and the purified gas was extracted from the top of the scrubber (T0103) tower. The CO_2-rich and H_2S-rich solvent entered the CO_2 desorption tower (T0104) after decompression flash evaporation. The gas stream obtained after flash evaporation is fed to the bottom of the scrubber tower (T0101) after compression heat transfer. In CO_2 desorption process, the majority of CO_2 is released from the desorption column. The rich solvent is subsequently transferred to H_2S-enriched stripper T0105, where CO_2 is desorbed by reducing operational pressure and facilitating N_2 stripping. The solvent then enters flash tank V0104, where H_2S and methanol are separated. The lean methanol solvent is collected at the bottom of the tower and directed to the low-temperature methanol scrubber for recirculation. The gas with a high H_2S concentration obtained at the top of the flash tank was sent to the sulfur recovery system.

2.1.4. MS and MD Unit.

Figure 7 illustrates the flowsheets for the MS and MD units. In the AGR section, the purified syngas is blended with the recycled gas before being introduced into the methanol synthesis reactor. Within this reactor, three key reactions take place utilizing a Cu/Zn/Al/Zr catalyst:[28]

$$CO + 2H_2 \rightarrow CH_3OH \qquad \Delta H_{298.15K} = 90.77\,\text{kJ/mol} \tag{13}$$

$$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O \qquad \Delta H_{298.15K} = 49.16\,\text{kJ/mol} \tag{14}$$

$$CO_2 + H_2 \rightarrow CO + H_2O \qquad \Delta H_{298.15K} = +41.21\,\text{kJ/mol} \tag{15}$$

After the WGS and AGR units, syngas is prepared for methanol synthesis. Water is removed through two pressurized flash evaporations, as shown in Figure 7. The syngas is then pressurized to 5.0 MPa and preheated to 200 °C before entering the synthesis reactor. Postreaction, the gas is cooled to 40 °C and sent to a flash tank to separate unreacted syngas. In the MS process, the separated gas is efficiently divided by a splitter, with approximately 10 wt % released as methanol gas in the Rectisol process.[21−23] The crude methanol extracted from the flash tank (PV-1) is subsequently routed to the rectification section for further processing. The distillation setup includes two columns: T-1, featuring 18 plates, and T-2, featuring 26 plates. Through two stages of distillation, methanol can achieve an impressive purity of 99.97 wt %.

Using the Rstoic model for reactor R-1, the Flash model for the flash tank, and the RadFrac model for the rectification tower, the feedstock gas flow rate was set at 3000 kmol/h, ensuring optimal performance across the system.[22,24]

2.1.5. MTO and Distillation.

The MTO process encompasses both the MTO unit and the subsequent separation and purification of light olefins. MTO unit is built on advanced DMTO technology,[30,31] ensuring efficient conversion. In this work, the RYield model is utilized to simulate the synthesis of olefins from methanol, while the RadFrac model is employed for simulating key components such as the cooling tower, washing tower, alkali washing tower, and predepropane separation tower, as shown in Figure 8. The HeatX model simulated a heat exchanger with a methanol conversion rate of 99.9% and olefins selection rate of 85%. Reaction conditions: 500 °C and 0.22 MPa. Final product purity: 99.97% ethylene and 99.98% propylene!

2.2. RE-CTO Route.

Compared with the conventional CTO route, renewable energy sources (such as wind and solar power) are introduced into pumps, heaters, and other utility equipment. This approach not only enhances sustainability but also aligns with our goal of reducing our carbon footprint.

Hydrogen production relies on renewable energy sources like wind, solar, hydropower, and nuclear.[32−34] To tackle the instability of these sources, we propose a hybrid energy system that reduces volatility.[35,36] Batteries are used for power storage,

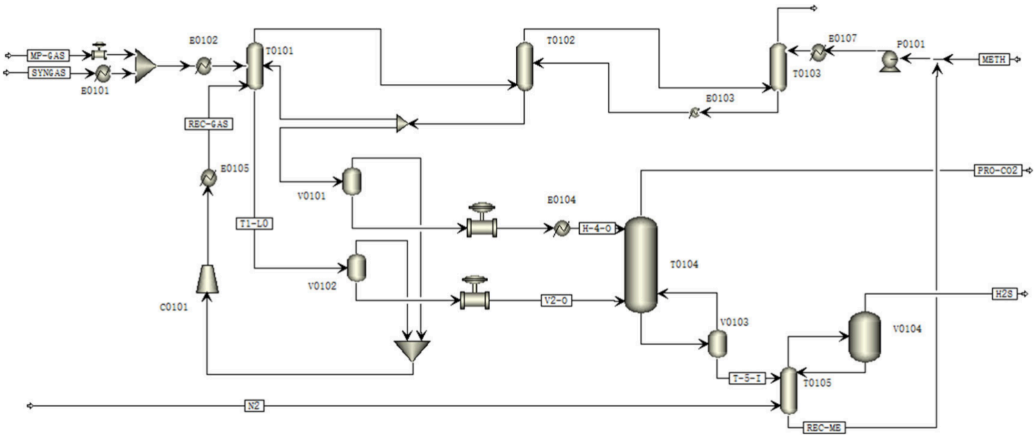

Figure 6. Process flowsheet of the AGR unit.

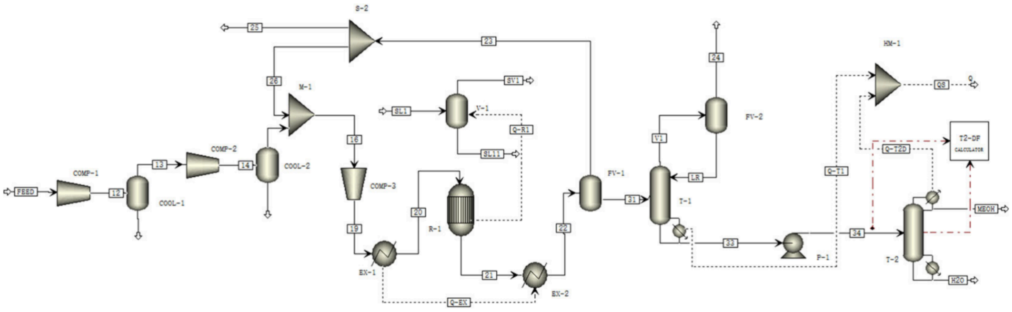

Figure 7. Process flowsheet for MS and MD unit.

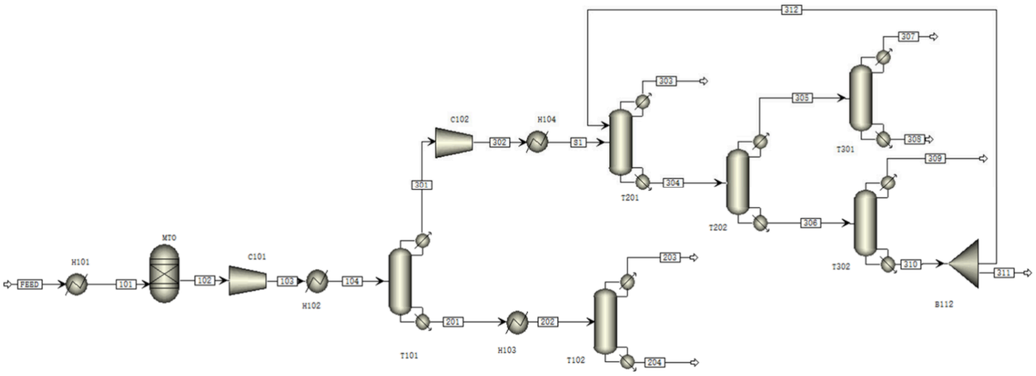

Figure 8. Process flowsheet for MTO and distillation.

supplying energy to the water electrolysis unit. Essential parameters of battery performance are detailed in Table 2.

Table 2. Essential Parameters of Battery Performance

parameter	value
type	lithium iron phosphate battery
charge cycle	2500 times
charge efficiency	90%
discharge efficiency	90%
single capacity	2.5 MWh
power of charge and discharge	0−0.3 MW

2.3. RE-GH-CTO Route.

The RE-GH-CTO route can eliminate the need for an air separation unit (ASU) and water−gas shift (WGS) unit. The system integrates the CG, AGR, MS, and MD units, with the (Power-to-Hydrogen) PtH unit supplying the oxygen needed for the CG unit, rather than relying on the ASU. In the methanol synthesis reactor, compressed hydrogen is introduced, where it reacts with CO and CO_2 to produce methanol.

The PtH equation illustrates a sustainable energy transformation:

$$H_2O + \text{renewable electricity} \rightarrow H_2(g) + \frac{1}{2}O_2(g) \tag{16}$$

In the realm of electrochemistry, the rate of hydrogen production through water electrolysis is directly proportional to the applied electric current. However, it is important to note that parasitic current losses can occur during this process. During electrolysis, demineralized water is heated, vaporized, and superheated, serving as the essential raw material for the cathodic reaction. To enhance the performance of the electrolytic material (Ni-YSZ) and prevent oxidation, we typically incorporate 10 vol % H_2 into the raw material gas. This addition significantly boosts the electrolytic conversion rate, achieving an impressive range of 85% to 90%.[37] The hydrogen production unit utilizes alkaline electrolyzers, recognized for their cost-effectiveness, established technology, and extensive industrial applications. For this study, we employed the RK-Soave thermodynamic method.[38] Table 3 provides a comprehensive overview of the key operational parameters of the electrolyzer.[39]

Table 3. Essential parameters of electrolyzer

parameter	value
power consumption production	51 kWh/kg H_2
working pressure	3.2 MPa
capacity of single electrolyzer	6 MW

The electrolyzer used in this study is a proton exchange membrane (PEM) electrolyzer, which is known for its high efficiency and scalability. The reported hydrogen energy consumption of 51 kWh/kg of H_2 is based on the specific operating conditions of our system, including elevated pressure and partial load operation. This value is consistent with literature reports for PEM electrolyzers under similar conditions.[40] The key operational parameters of the conventional CTO route are illustrated in Table 4.

3. SIMULATION RESULTS

In the conventional CTO route, 277.22 t/h coal uses 138.61 t/h of O_2 to generate 261.84 t/h crude syngas. Post-WGS reaction yields 91.91 t/h of CO, 14.07 t/h of H_2, and 141.12 t/h of CO_2. The Rectisol unit captures 135.81 t/h of CO_2 for storage, whereas in the RE-GH-CTO route, CO_2 serves as feed gas. In the MS unit, 163.23 t/h CO, 5.31 t/h CO_2, and 23.78

Table 4. Key Operational Parameters of the CTO Route

unite	physical property method	key parameter	value
AS		mole purity level O_2	99.9%
		mole purity level N_2	97.4%
CG	RK-SOAVK	gasification pressure	0.2 MPa
		gasification temperature	1554 °C
WGS	NRTL	pressure	3.2 MPa
		shift ratio	60%
AGR	PSRK	pressure	3.3 MPa
		temperature	−50 °C
MS	RK-SOAVK	reaction temperature	200 °C
		pressure	5.0 MPa
MD	NRTL	methanol purity	99.9%
MTO		reaction temperature	500 °C
		pressure	0.22 MPa
OD	NRTL	ethylene purity	99.9%
		propylene purity	99.9%

t/h H_2 are utilized to synthesis methanol. Following the distillation process, a high-purity methanol product with 99.9 wt % is obtained, with a production rate of 22.85 t/h (equivalent to 6983.29 kmol/h). After the MTO and light olefin distillation, 37.03 t/h ethylene and 36.18 t/h propylene were obtained. The CTO and RE-CTO routes have the same unit operations of chemical engineering, but electricity is sourced from different origins. The electricity is derived from thermal power generation in the conventional CTO route, while the electricity in the RE-CTO route originates from renewable energy generation. For the RE-GH-CTO route, 138.61 t/h O_2 and 17.32 t/h H_2 are provided by the PtH unit. The AGR unit effectively removes nearly 100% of H_2S, while supplying 9.47 t/h of renewable green hydrogen to the MS unit, ensuring an optimal hydrogen-to-carbon ratio. Subsequently, 248.48 tons of methanol is obtained with the same amount of coal as the raw material, which is 1.13 times the amount of methanol produced by conventional CTO. The simulation results of the CTO and RE-GH-CTO route are presented in Table 5.

4. RESULTS AND DISCUSSION

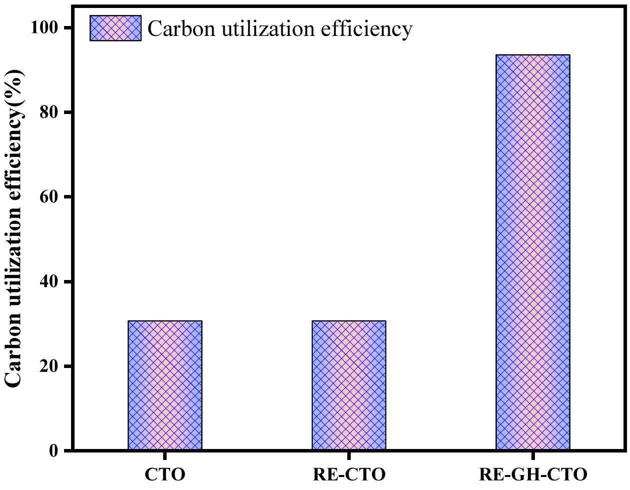

Figure 9. Carbon utilization efficiencies of CTO, RE-CTO, and RE-GH-CTO.

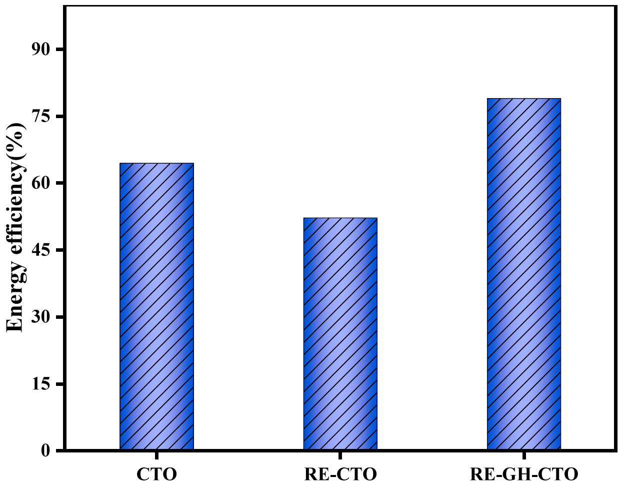

Figure 10. Energy efficiency for the CTO, RE-CTO, and RE-GH-CTO route.

4.1. Carbon Utilization Efficiency. Carbon utilization efficiency is a critical metric for the CTO, RE-CTO, and RE-GH-CTO routes. In the CTO route, an impressive 99.19% of carbon in coal is transformed to CO and CO_2. After the WGS and AGR units, approximately 57.48% of the carbon is further

Table 5. Results for Main Streams of the Conventional CTO and RE-GH-CTO Route

	CTO			RE-GH-CTO		
stream	crude syngas	Rectisol	MTO	crude syngas	Rectisol	MTO
N_2	0.0109	0.2067	0	0	0	0
O_2	5.75×10^{-16}	0	0	5.75×10^{-16}	0	0
H_2O	2.23×10^{-7}	0	0	2.23×10^{-7}	0	0
CO	0.8327	0.6729	0	0.8327	0.6903	0
CO_2	1.16×10^{-7}	0.0219	0	1.16×10^{-7}	0.0355	0
H_2S	0.0070	0	0	0.0070	0	0
H_2	0.0349	0.0980	0	0.0349	0.2703	0
CH_3OH	0	0	0.008	0	0	0.008
$C_2H_4 + C_3H_6$	0	0	0.99	0	0	0.99
mass flow (kg/h)	261814.77	242549.00	73948.50	262420	242549.00	83956.46

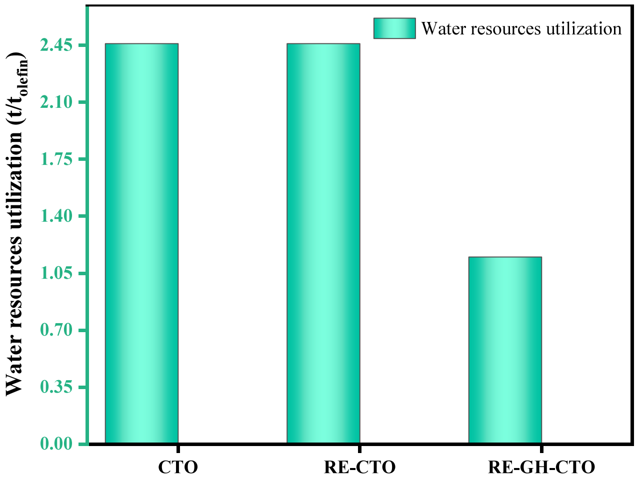

Figure 11. Water resource utilization for the CTO, RE-CTO, and RE-GH-CTO routes.

Table 6. Ratio Factor of the Component of FCI[a]

item	suggestion percentage	RF
1. Direct investment		
1.1. Equipment	15%−40% of FCI	40
1.2. Installation	6%−14% of 1.1	12
1.3. Instruments and controls	2%−8% of 1.1	6
1.4. Piping	3%−20% of 1.1	15
1.5. Electrical	2%−10% of 1.1	10
1.6. Buildings (including services)	3%−18% of 1.1	15
1.7. Land	1%−2% of 1.1	1
2. Indirect investment		
2.1. Engineering and supervision	4%−21% of direct investment	18
2.2. Construction and contractor expenses	6%−22% of direct investment	15
2.3. Contingency	5%−15% of FCI	15
3. Fixed capital investment	direct + indirect investment	100

[a] Data taken from ref 46.

Table 7. Equipment Investments in Three Routes

	Investment Cost (× 10^8 CNY)		
item	CTO	RE-CTO	RE-GH-CTO
air separation unit	3.37	3.37	
gasification unit	11.51	11.51	11.51
WGS unit	0.55	0.55	
AGR unit	2.34	2.34	
MS and MD unit	5.65	5.65	5.65
MTO unit	13.84	13.84	13.84
electric power system		1.50	1.50
PtH unit			2.50
total equipment investment	37.60	38.76	35.00

Table 8. Ratio Factors of Production Cost

item	basis
(1) Raw material	See Table9
(2) Utilities	See Table9
(3) Operating and Maintenance	
(3.1) Operating labor	100 000 CNY/labor/year
(3.2) Direct supervisory and clerical labor	10% of 3.1
(3.3) Maintenance and repairs	2% of FCI
(3.4) Operating supplies	0.7% of FCI
(3.5) Laboratory charge	1.5% of 3.1
(4) Depreciation	life period 20 years, salvage value 4%
(5) Plant overhead cost	60% ((3.1) + (3.2) + (3.3))
(6) Administrative cost	2% of production cost
(7) Distribution and selling cost	2% of production cost
(8) Production cost	(1) + (2) + (3) + (4) + (5) + (6) + (7)

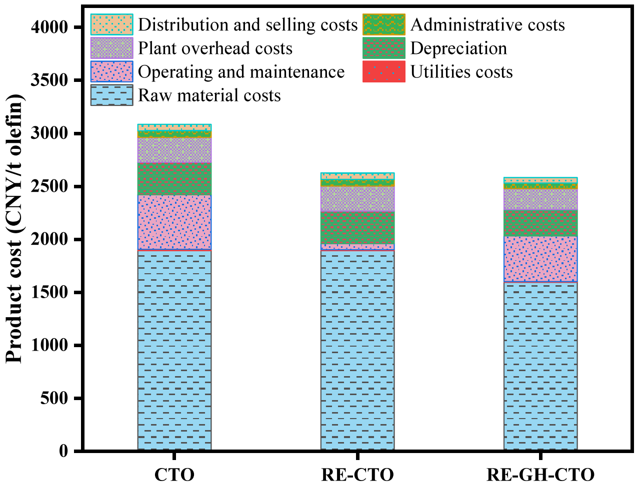

Figure 12. Production costs for the CTO, RE-CTO and RE-GH-CTO routes.

Table 9. Current Pricing Trends for Raw Materials and Products (CNY/t)[a]

item	price	item	price	item	price
coal	500	ethylene	8800	cooling water	2
natural gas	2800	propylene	7600	HP steam	210
H_2	10 000	ethane	3600	MP steam	106
CO_2	300	C_4 fraction	5000	LP steam	88
methanol	2100	process water	15	thermal power[b]	0.70
renewable electricity[b]	0.40				

[a] Data taken from ref 47. [b] The unit of electricity is CNY/(kW h).

converted to CO_2, which is then effectively separated from clean syngas, and a production rate of approximately 73 209 kg/h of light olefins through the CTO route. For the RE-GH-CTO route, this innovative method allows for the loss of only 0.99% of carbon from clean syngas, while an impressive 97.52% of carbon is effectively utilized in the production unit of MS and MTO, resulting in a total output of 222 877 kg/h of light olefins, as shown in Figure 9. Notably, the carbon utilization efficiency of the RE-GH-CTO route has been significantly enhanced, increasing from 30.74% to an outstanding 93.58%, compared to the conventional CTO route. The RE-GH-CTO route boosts carbon utilization efficiency by an impressive 3.04 times, compared to the traditional CTO route. This innovative approach is a game-changing tool for enhancing carbon efficiency. This advancement not only highlights the potential for improved sustainability in olefin production but also reduces carbon emissions in the industry.

The CTO and RE-CTO routes not only share identical coal processing capacities but also deliver consistent quality in light olefins. Additionally, the oxygen generated as a byproduct of the PtH process fully satisfies the needs of the CG unit in the

RE-GH-CTO route. Consequently, the need for the air separation unit is eliminated, thereby saving significant investments and reducing energy consumption associated with operating that equipment.

4.2. CO_2 Emissions. The CO_2 emissions for CTO, RE-CTO, and RE-GH-CTO routes have been analyzed. In addition to direct CO_2 emissions, indirect CO_2 emissions should be considered. Together, these factors contribute to the overall carbon footprint, highlighting the importance of addressing both direct and indirect emissions in our sustainability efforts.[41,42] The analysis reveals that the direct emissions for the CTO, RE-CTO, and RE-GH-CTO routes are 5.7, 3.2, and 0.03 t of CO_2/t of olefin, respectively. In contrast, the RE-GH-CTO route achieves a remarkable milestone: it operates with net-zero carbon emissions.

In this analysis of heat recovery and energy consumption, it is found that the CO_2 emissions for the CTO, RE-CTO, and RE-GH-CTO routes are 11.25, 5.4, and an impressive 0.12 t CO_2/t olefin, respectively. This highlights the RE-GH-CTO route as a highly effective solution for significantly reducing greenhouse gas (GHG) emissions.

4.3. Energy Efficiency. The energy efficiencies of the CTO, RE-CTO, and RE-GH-CTO routes were investigated.[43,44] The energy efficiencies of these three routes were calculated using eq 25.

$$\phi = \frac{E_{\text{Olefin}}}{E_{\text{Coal}} + E_{\text{Util}}} \qquad (25)$$

where ϕ denotes the energy efficiency in CTO, RE-CTO, and RE-GH-CTO routes, E_{Olefin} denotes energy in the olefin products, E_{Coal} denotes energy in coal, and E_{Util} is the energy input from utilities (e.g., steam and electricity).

Figure 10 discloses the energy efficiency of the CTO, RE-CTO, and RE-GH-CTO routes. In the CTO route, the production of 1 kg of olefin consumes 3.79 kg of coal and 43.16 MJ of energy. The energy efficiency of the CTO route was calculated to be 64.45%. The energy efficiency is calculated on the grounds of the lower heating values of coal, H_2, ethylene, and propylene (20.9 MJ/kg, 9.7 MJ/m^3, 14 197 kcal/m^3, 20 925 kcal/m^3, respectively).[42] In the RE-GH-CTO route, the production of 1 kg of olefins requires 1.24 kg of coal, 0.10

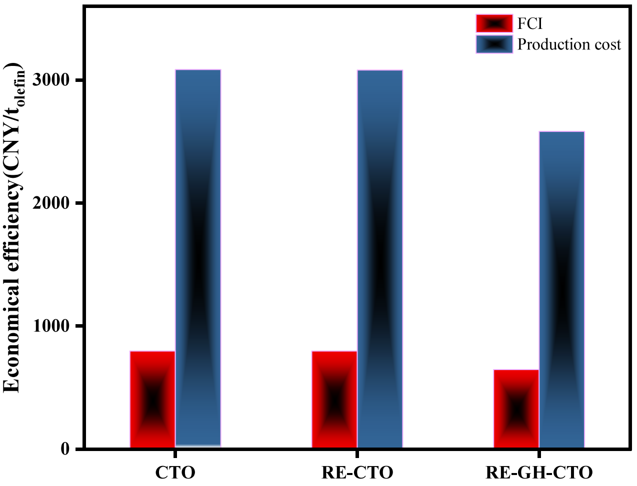

Figure 13. Production costs and FCI for the CTO, RE-CTO, and RE-GH-CTO routes.

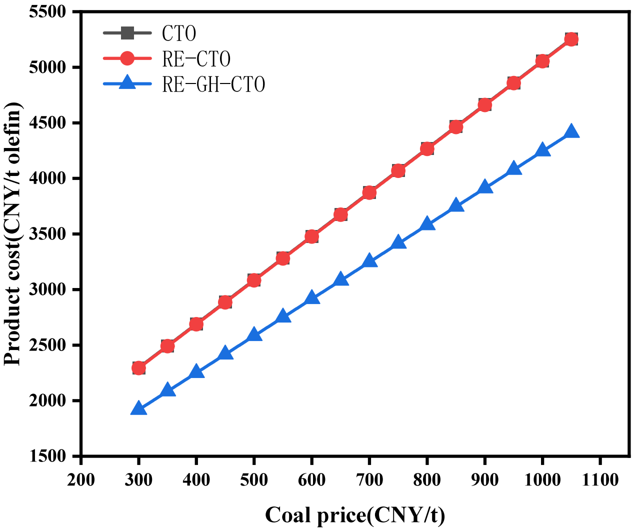

Figure 14. Coal price and product cost for the CTO, RE-CTO, and RE-GH-CTO routes.

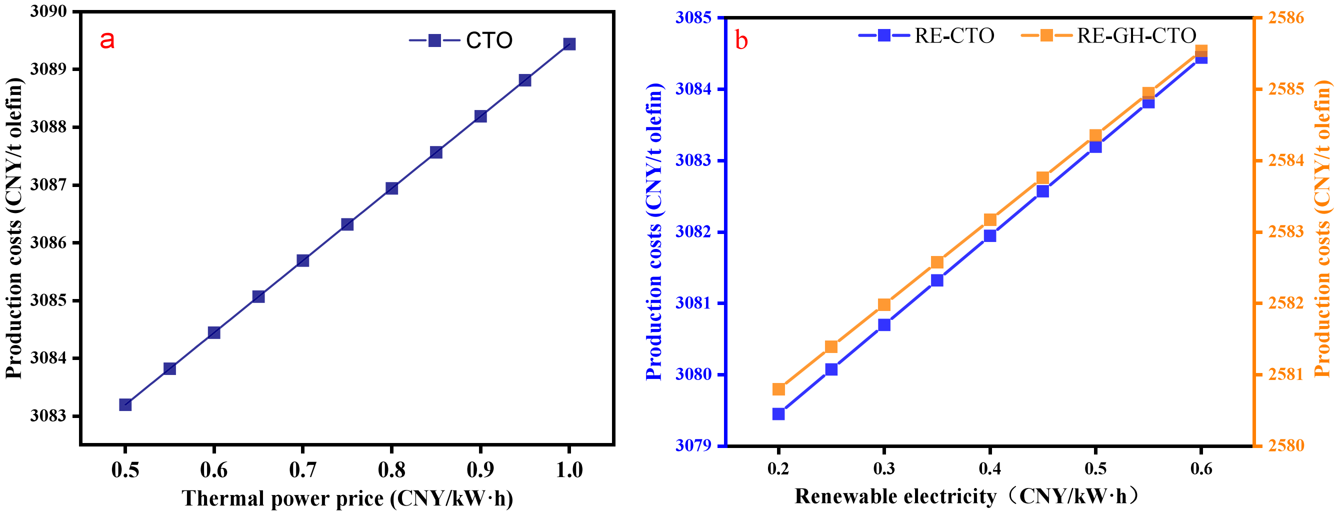

Figure 15. (a) Thermal power price and product cost for the CTO routes; (b) renewable electricity price and product cost for the RE-CTO and RE-GH-CTO routes.

kg of H_2 and 15.97 MJ of energy. The energy efficiency was 78.99% for the RE-GH-CTO route. Considering the charge and discharge loss of green electricity, therefore, the charging and discharging efficiency of green electricity in the RE-CTO and RE-GH-CTO routes should be taken into account, as shown in Table 2. The energy efficiency of the three routes can be calculated according to eq 25 and the lower heating values of each raw material, as shown in Figure 10. The energy efficiency of the three light olefins production routes of CTO, RE-CTO, and RE-HG-CTO were 64.45%, 52.20%, and 78.99%, respectively. The RE-HG-CTO route was 14.51% more energy efficient than the CTO route.

4.4. Water Resources Utilization. The route of CTO comprises two stages: coal to methanol (CTM) and methanol to olefin (MTO). The water consumption primarily occurs in the CTM stage, and the byproduct of methanol to olefin is 0.56t water/t olefin. Compared to the conventional CTO route, the RE-GH-CTO route eliminates the need for the WGS unit, thereby resulting in water savings. However, it introduces an electrolytic water unit, which consumes water during the electrolysis process. It is important to consider both the water-saving benefits and the water utilization associated with the different units throughout the overall process.

The water utilization was calculated according to the water utilization per unit product output, as shown in Figure 11. First, in the simulation route of the RE-GH-CTO, there was the electrolytic water unit, which indeed required a large amount of water utilization as raw materials. From this point of view, the water utilization was increased. Second, the product outputs of the RE-GH-CTO route were increased; as the denominator, the water utilization per unit product output was relatively reduced. Third, in the reaction of methanol synthesis of olefin, part of the byproduct water, the proportion of this part of the water in the product was about 55.4%,[45] and this part of the byproduct water was used as a supplement for circulating water, which would alleviate the part of the water utilization. In summary, when considering the water generation as byproduct in MTO unit, the overall water utilization of CTO, RE-CTO, and RE-GH-CTO routes are 2.46, 2.46 and 1.15t/t olefin, respectively. However, the overall water utilization of CTO, RE-CTO, and RE-GH-CTO routes are 144.15, 144.15, and 204.73 t/y. Therefore, the RE-GH-CTO route can relatively reduce water utilization in terms of the water utilization per unit product output. In terms of water utilization per unit of olefin production, the RE-GH-CTO route has the clear advantage of saving water.

Indeed, in the operation of the coal gasification unit, both the CTO and RE-GH-CTO routes exhibit similar water utilization. However, the electrolytic water unit for hydrogen production requires a significant amount of water, resulting in higher total water utilization in the RE-GH-CTO route. As a result, implementing the RE-GH-CTO route in coal-rich areas that are already characterized as arid or semiarid can present substantial challenges. The water scarcity in such regions could limit the feasibility and sustainability of the RE-GH-CTO route. Therefore, it is crucial to carefully evaluate the water availability and potential impacts on local water resources before implementation of the process in these areas. Additional measures may need to be taken to address the water utilization challenges and ensure the process's viability in such water-limited environments.

4.5. Economic Performance. *4.5.1. Fixed Capital Investment.* The fixed capital investment (FCI) serves as a key indicator of the economic performance for the CTO, RE-CTO, and RE-GH-CTO routes. It includes a comprehensive range of components such as equipment, installation, piping, instrumentation and controls, electrical systems, land, buildings, engineering, construction, legal, and contractor fees, as well as project contingencies. The equipment investment is detailed in Table 6.

Taking the annual production scale of 600 000 tons of light olefins as an example, the equipment investment of the three light olefins production routes is shown in Table 7. The FCI for the CTO, RE-CTO, and RE-GH-CTO routes is 797.59, 797.59, and 646.41 CNY/t olefin, respectively, as shown in Figure 13. The FCI for RE-GH-CTO route is approximately 23.39% lower than that of the CTO and RE-CTO route.

4.5.2. Production Cost. The corresponding economic assumptions are shown in Table 8 and Figure 12. In calculating the depreciation cost, a depreciation life of 20 years and a residual value rate of 4% are assumed. Additional product costs are estimated using a ratio estimation approach. All costs are presented in the CNY.

Figure 13 illustrates the production costs and FCI for the CTO, RE-CTO, and RE-GH-CTO routes. The production costs for the CTO, RE-CTO, and RE-GH-CTO routes are 3085.69, 3081.94, and 2583.17 CNY/t olefin, respectively. The production cost of the RE-GH-CTO route demonstrates superior economic performance, compared to the other processes.

4.6. Sensitivity Analysis. The effects of coal price, thermal power price, and renewable electricity price on the production cost of light olefins were investigated by sensitivity analysis. Light olefins production costs were affected by coal price fluctuations, as shown in Figure 14.

The thermal power price fluctuation range was 0.5−1.0 CNY(/(kW h), the renewable electricity price fluctuation range was 0.2−0.6 CNY/(kW h), snd the coal price fluctuation range was 300−1100 CNY/t. The thermal power price has a great direct correlation with the coal price. In addition, the growth of renewable electricity on scale would also affect the overall power price. Therefore, in the sensitive analysis, the correlation between renewable electricity prices, thermal power prices, and coal prices were considered. Figure 15 revealed the impact of the electricity price on the production cost of light olefins of the three routes. With the increasing of electricity prices, the production cost of light olefins increased. However, the electricity prices were driven by policy regulations, technological progress and market supply and demand. With the progress of technology, the production costs of electricity would gradually decrease.

According to the market price, in the Xinjiang region of China, the civil electricity price is 0.39 CNY/(kW h), and the Chinese government strongly encourages the development of renewable electricity, preferential policies, and government subsidies make green electricity price may be even lower. Industrial electricity prices generally ranged from 0.6 CNY/kW h to 1.0 CNY/kW h in China; electricity prices changed due to different periods of electricity consumption, especially high energy consumption enterprises, or peak electricity prices may be close to or more than 1.0 CNY/(kW h).

5. CONCLUSIONS

This study proposes a novel sustainable production of light olefins coupling renewable electricity and green hydrogen to achieve low CO_2 emissions and high olefin production rates.

The green hydrogen is provided by the PtH unit in the novel olefins production route to adjust the H/C ratio. The RE-GH-CTO route eliminates the WGS unit to reduce CO_2 production at the bottom, improves carbon efficiency, increases light olefin productivity and economics, and reduces environmental impact. The key conclusions of this study are as follows.

The energy efficiency for the RE-GH-CTO route is 14.51% higher than the conventional CTO route, while the CO_2 emission is net-zero compared to that of the CTO route. The RE-GH-CTO route demonstrates a remarkable 77.51% reduction in water resource utilization compared to the conventional CTO route. The production cost of RE-GH-CTO route is 19.31% lower than that of the CTO route. Additionally, the FCI in the RE-GH-CTO route is approximately 23.38% lower, compared to the CTO and RE-CTO routes.

The RE-GH-CTO route offers a viable approach to sustainable coal-to-chemical conversion because of the improved CO_2 utilization efficiency resulting from the introduction of green hydrogen. This work can provide new ideas for the future development of clean and efficient energy technologies and ultimately achieve carbon-neutral sustainable development.

■ ASSOCIATED CONTENT

Data Availability Statement

Data will be made available on request.

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Notes

The authors declare no competing financial interest.

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■ NOMENCLATURE

ASU = air separation unit
AGR = acid gas removal
CCS = carbon capture and storage
CG = coal gasification
CTM = coal-to-methanol
CTO = coal-to-olefin
DMTO = dimethyl ether/methanol-to-olefins
FCI = fixed capital investment
GH = green hydrogen
GHG = greenhouse gas
H/C = hydrogen-to-carbon
HPS = high-pressure steam
RE-CTO = Renewable Electricity Integrated with Coal-to-Olefin Process
RE-GH-CTO = Renewable Electricity and Green Hydrogen Integrated with Coal-to-Olefin Process
MD = Methanol Distillation
MS = Methanol Synthesis
MS&D = Methanol Synthesis and Distillation
MTO = methanol-to-olefin
NG = natural gas
OD = olefin distillation
PtH = power-to-hydrogen
SR = sulfur removal
WGS = water-gas shift

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