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3 **Techno-economic analysis of coal-to-liquid processes**
4 **with different gasifier alternatives**

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Abstract

Considering the current national conditions of China, developing coal-to-liquid process is an attractive way to alleviate the domestic oil crisis. Coal-to-liquid process mainly includes six subsystems and the most essential unit of the system is the gasification unit. This paper aims to provide suggestions for the cleaner production and sustainable development of coal-to-liquid technology Lurgi, Texaco and Shell coal-to-liquid process are modelled and simulated. The techno-economic analysis is conducted to investigate their performance using simulation-based results. Results showed that the greenhouse gas emissions of Lurgi, Texaco, and Shell coal-to-liquid process are 5.26 t/t fuel, 4.86 t/t fuel, and 3.49 t/t fuel. Lurgi coal-to-liquid has better performance on reducing oxygen cost and total investment; Texaco coal-to-liquid is advantageous in saving steam cost and production cost; Shell coal-to-liquid shows better performance in terms of energy efficiency, reducing the consumption of coal and water, and greenhouse gas emission. Shell gasifier is recommended in water-deficient areas. Texaco gasifier is recommended when access to water and coal is sufficient. Lurgi gasifier is recommended in pilot-scale projects. In the view of sustainable development, Shell gasifier is prior to Texaco gasifier and Lurgi gasifier because of the low greenhouse gas emission and well resistance to high coal price and high carbon taxes. Gasification unit occupies the largest proportion of total capital investment of coal-to-liquid processes and significantly affects the syngas composition. Coal gasification technology is potentially limiting the overall acceptance and practice of coal-to-liquid process in the future.

Keywords: Lurgi gasifier; Texaco gasifier; Shell gasifier; techno-economic analysis.

1 Nomenclature

2	CTL	coal-to-liquid
3	CBTL	coal biomass to liquids
4	WGS	water gas shift
5	STL	shale-to-liquid
6	GHG	greenhouse gas emission
7	ASU	air separation unit
8	LPG	liquefied petroleum gas
9	VLE	vapor-liquid equilibria
10	F-T synthesis	Fischer-Tropsch synthesis
11	LHV	lower heating value
12	η	energy efficiency (%)
13	E_P	energy of the fuel (GJ)
14	E_T	total energy consumption (GJ)
15	ϕ_{cc}	coal consumption (t/t fuel)
16	m_P	weight of fuel (t)
17	m_C	weight of coal (t)
18	ϕ_{wc}	water consumption (t)
19	m_w	weight of water (t)
20	ϕ_{Oc}	oxygen consumption (Nm ³ /t fuel)
21	V_O	standard volume of consumed oxygen (Nm ³)
22	ϕ_{sc}	steam consumption (GJ/t fuel)
23	E_S	energy of all steam (GJ)
24	I_1	equipment investment of the reference project (CNY)
25	I_2	equipment investment of the studied project (CNY)
26	Q_1	scale of the reference project

1	Q_2	scale of the studied project
2	sf	scale exponent
3	TCI	total capital investment (CNY)
4	EI	equipment investment (CNY)
5	i	components of the investment
6	RF	ratio factor (%)
7	PC	production cost (CNY/t fuel)
8	C_R	raw material cost (CNY/t fuel)
9	C_U	utility cost (CNY/t fuel)
10	$C_{O\&M}$	operating and maintenance cost (CNY/t fuel)
11	C_D	depreciation cost (CNY/t fuel)
12	C_{POC}	plant overhead cost (CNY/t fuel)
13	C_{AC}	administrative cost (CNY/t fuel)
14	C_{DSC}	distribution and selling cost (CNY/t fuel)
15	m_{CO_2}	annual carbon emission (t/y)
16	m_{LPG}	annual production of liquefied petroleum gas (t/y)
17	m_{Diesel}	annual production of diesel (t/y)
18	$m_{Naphtha}$	annual production of naphtha (t/y)
19	$PC_{carbon-tax}$	production cost considering carbon tax (CNY/t fuel)
20	$f_{Carbon-emission}$	carbon emission (t/t fuel)
21	CT	carbon tax (CNY/t)

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1. Introduction

The richness in coal while a shortage of oil and gas are the current energy resource distinctive features in China (Zhou et al., 2016). The coal reserve is as high as 5.9×10^{12} t, accounting for 94% of the total energy resources of China. Oil and natural gas resources occupy only 6% of the total energy resources (National Development & Reform Committee of China, 2007; 2009), which are also difficult to increase their production. Gasoline and diesel consumption has increased years in China (Lu et al., 2014). In 2017, the oil production of China was 192 Mt, while the oil consumption of China is 590 Mt (MLR, 2017). It can be easily obtained that 67.4% consumed oil in China relies on import from foreign countries. It was reported that the demand for oil had exceeded 600 Mt for the first time in 2018, reaching 615 Mt. And the foreign dependence will approach 70%. The oil and natural gas in China highly depend on import from other countries, where foreign dependence will approach 70%. There are several routes to produce gasoline and diesel, for example, coal (Leckel et al., 2011), biomass (Perego et al., 2009), natural gas (Choudhury et al., 2015), waste (Hazrat et al., 2014), etc. Based on the current national conditions of China, developing coal-to-liquid (CTL) can alleviate the oil crisis of China. However, the development of CTL industry is facing the severe test of resource supply, demand and pollution emission. The National Climate Change Plan (2014-2020) points out that, China will achieve the goal of reducing carbon dioxide emissions per unit GDP by 40-45% by 2020 compared with 2005 (National Development & Reform Committee of China, 2014). The cleaner production and robust development of CTL will be an important way to achieve the goal.

The CTL typically includes six subsystems, including the gasification unit, the air separation unit, the water gas shift unit (WGS), the Rectisol unit, the F-T synthesis unit, and the hydrotreating and separation unit (Williams et al., 2003). The most essential unit in CTL subsystems is the gasification unit. Coal gasification was developed more than decades ago. Fixed bed gasifier, fluidised bed gasifier, and entrained bed gasifier are

1 widely industrialised in the large-scale commercial plant (Yang et al., 2017). In these
2 gasification technologies, Lurgi gasifier, Texaco gasifier, and Shell gasifier have been
3 successfully applied to the CTL process in China (Tian et al., 2006).

4 A cleaner production and robust development for CTL require a comprehensive and
5 broad assessment. Rafati et al. (2017) investigated the main operation parameter effects
6 on energy efficiency and the economic performance of biomass to liquid. Chiodini et al.
7 (2017) reported a new approach to biomass gasification and aimed to set up more
8 efficient biomass to liquid process. Snehesh et al. (2017) studied a technical analysis
9 (including oxygen to steam ratio, steam to biomass ratio, etc.) on biomass to liquid by
10 Fisher-Tropsch route. Ramberg et al. (2017) studied the economic viability of natural gas
11 to liquid and examined the evolution of the natural gas price. Many researchers were
12 focused on the techno-economic performance of CTL process. Zhou et al. (2016)
13 modelled and simulated a STL and a CTL and compared their techno-economic
14 performance. The results provided suggestions for improving economic performance and
15 energy efficiency of the CTL and STL. In addition, comparison of life cycle greenhouse
16 emissions and water consumption of the CTL and STL were compared (Zhou et al.,
17 2019). Zhou and co-workers simulated CTL process and three CO₂ capture alternatives
18 and compared three CO₂ capture methods in terms of economic and energy performance
19 (Zhou et al., 2011). Jiang et al. (2017) performed four different configurations of direct
20 coal biomass to liquids (CBTL) and conducted techno-economic analysis. Results
21 revealed that the utilization of shale gas can enhance the performance of direct
22 liquefaction process compared with indirect CBTL. Mohajerani et al. (2018) compared
23 the techno-economic performance of a CTL and a gas-to-liquid (GTL) by the scale factor
24 method. Results showed that the scale-up factors of CTL and GTL were estimated to 0.65
25 and 0.70. Zhou et. (2018) Conducted the economic and exergy analysis of CTL coupling
26 carbon dioxide capture and storage for five different coal types. Results suggested that
27 gas coal can achieve the better performance on cost and exergy utilization. Mapamba et

al. (2017) investigated the economic performance impact of plasma arc reforming deployment on CTL. Results showed that the plasma arc reforming deployment has a positive impact on the economic performance of CTL. Qin et al. (2018) compared the energy, exergy and technoeconomic performance of different entrained flow gasifier alternatives. According to Xu et al. (2015), it is reported that the Lurgi, Texaco, and Shell gasifiers have been industrialized in China.

For a cleaner production and robust development for industrialized CTL in China, Lurgi CTL, Texaco CTL, and Shell CTL are extensively modelled and simulated in this paper. The techno-economic analysis is conducted and compared based on simulation results. This research aims to provide suggestions for the cleaner production and sustainable development of CTL technology. The comparison results can guide future industrial improvements and CTL investments. Section 2 gives a detail description of CTL. Simulations with different gasification alternatives are conducted in this part. Comparisons of Lurgi CTL, Texaco CTL, and Shell CTL are presented in section 3, considering energy efficiency, material consumption, utility cost, total capital investment, production cost, and GHG emission. Conclusions in this work are given in section 4.

2. Process description and simulation

2.1 Process description

The block diagram of CTL is shown in Fig. 1. Coal is firstly fed into the gasification unit with steam and O_2 generated from an air separation unit (ASU). The crude gas mixture mainly composed of CO and H_2 is then produced by the gasification unit and subsequently cooled and washed, where the trace components are removed. Depending on whether adjustment of the hydrogen to carbon ratio in the shift gas to meet the requirement of F-T synthesis, a WGS unit may be employed. As a result of shift reactions, in WGS unit, the concentration of CO_2 is increased, followed by the shift gas fed into Rectisol unit to remove H_2S and CO_2 . Hydrocarbon liquids are synthesised by the purified gas from the Rectisol unit in the F-T synthesis reactor. Following the conversion

reactions, the liquids leave the F-T synthesis unit and are processed into hydrotreating and separation unit, where liquefied petroleum gas (LPG), naphtha and diesel are produced.

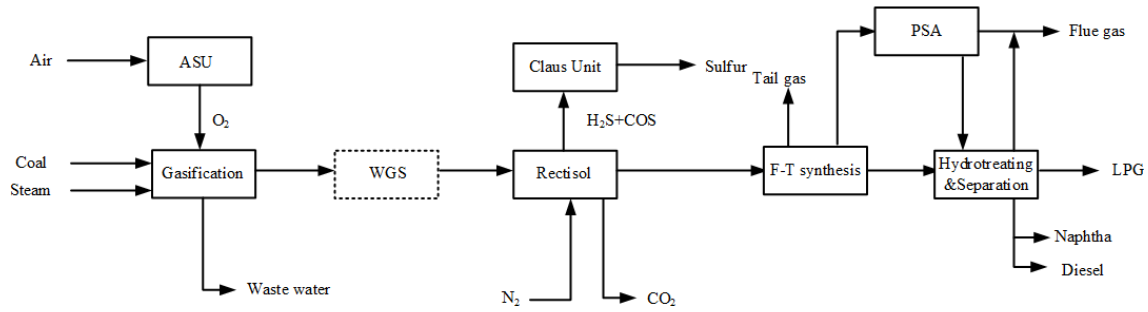


Figure 1. Process diagram of CTL

2.1.1 ASU

The schematic diagram of the ASU is shown in Fig.2. High purity O₂, which is the oxidant of the gasification unit, is provided by ASU. Cryogenic air separation was adopted in this work. Firstly, the air is pressurised by the air compressor and cleaned by the molecule sieve. The treated air is fed into a separation tower, where produces high purity O₂ from N₂ and Ar. The purity of O₂ is reached 95% (mol), which is sent to the gasification unit and the clause unit used as an oxidant. The stripping gas is high purity N₂, which is used in the Rectisol unit or sweeping gas in the CTL process.

2.1.2.1 Lurgi gasification

Lurgi gasifier is a kind of fixed bed gasifier (Xu et al., 2006), which is a vertical countercurrent reactor and shown in Fig. 3. Coal is fed into the gasifier at the top. The oxidant is a mixture of oxygen and steam, which is fed into the gasifier at the bottom. The coal moves downward under the force of gravity, while the oxidant moves upward under the force of pressure. In the process of countercurrent contact, coal reacts with the oxidant. These reactions occur in the sequence of coal drying, coal pyrolysis, char gasification, and char combustion (Hobbs et al., 1992). Solid wastes conclude that unreacted char and ash are removed at the bottom of the gasifier. The crude syngas consists of CO_2 , CH_4 , H_2 , CO , and other hydrocarbons leaves at the top of the gasifier.

The Lurgi gasifier was modelled in Aspen Plus by gasification section, pyrolysis section, and drying section. RK-SOAVE was selected as the thermodynamic method. RYield block and RCSTR block were used to simulate the reactions. The details of the simulation have been introduced in the previous publication (Yang et al., 2017).

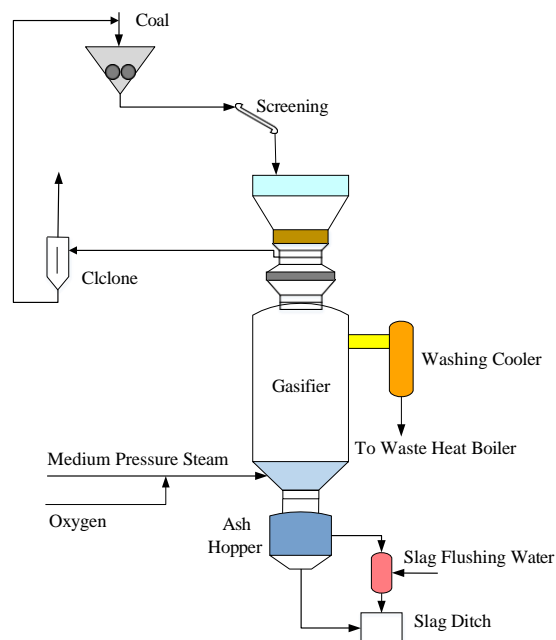


Figure 3. Schematic diagram of Lurgi gasifier

2.1.2.2 Texaco gasification

Texaco gasifier is a typical entrained flow bed gasifier (Lee et al., 2010), which is presented in Fig. 4. The feedstock is a coal-water slurry that is a mixture of coal and water. The mixture is pressurised and fed into the gasifier. The slurry reacts with the high purity O_2 at 40 bar. Coal pyrolysis, volatile combustion and char gasification reactions take place subsequently to produce the crude gas. The temperature of the crude gas is approximately 1,250 °C. A reservoir of water is maintained at the bottom of the gasifier by continuous injection of cooling water. The slag and crude gas leaving the gasifier pass through a water-cooled dip tube into the water reservoir. The slag remains in the water and then is removed. The crude gas is saturated with water and removed from the gas space above the water.

For modelling this unit, coal is converted into conventional elements, which can be treated in Aspen Plus. RGibbs model was employed to simulate the gasification. The simulation result was compared with the output of the composition published in the work of Xiang et al. (2014). The calculated results show a good agreement to the referenced values.

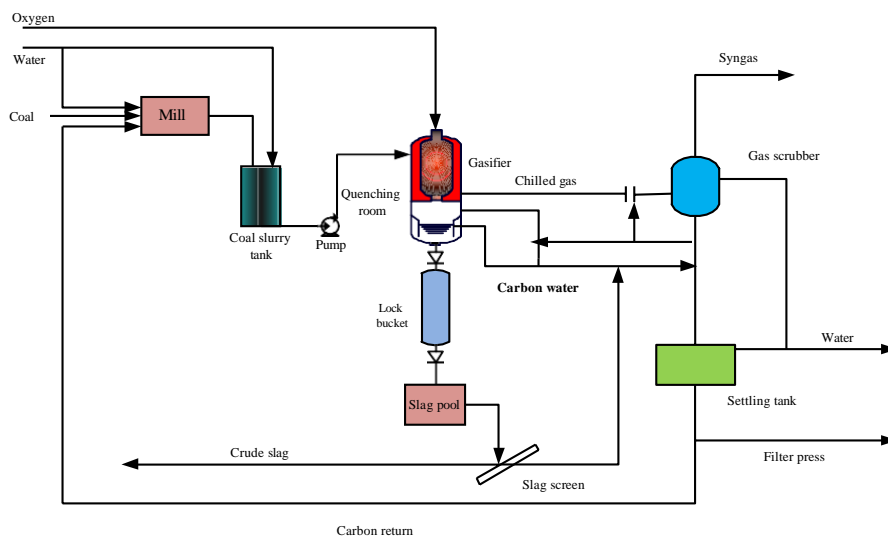


Figure 4. Schematic diagram of Texaco gasifier

2.1.2.3 Shell gasification

Shell gasifier is a typical entrained flow bed gasifier, which is illustrated in Fig. 5. The feed to Shell gasifier is dry pulverised coal, which is less sensitive to coal rank, compared to Lurgi gasifier and Texaco gasifier. After pulverised, the coal is dried, which is containing 2%-10% residual moisture. The dried coal is carried by nitrogen, where the mixture is pressurised. The pressurised coal is fed into the bottom of the gasifier with oxygen. The coal reacts with the oxygen and decomposes into volatile matters and char particles. After devolatilization, the char particles continue to react with the oxidant, where occurs various heterogeneous and homogeneous reactions. The product of the various reaction is mixed with volatiles matters. The mixture gas is the syngas and leaves at the top of Shell gasifier (Jeog et al., 2017).

For modelling this unit, the method is similar to the modelling of Texaco gasification. Coal is decomposed to conventional elements, which is represented by single element molecules (C, H, O, N, S, Cl, etc.) and ash (nonconventional element). RGibbs model is employed to simulate the gasification. The model was verified by the crude gas composition reported by Liu et al. (2014). The simulated result shows a small relative error to the reference data.

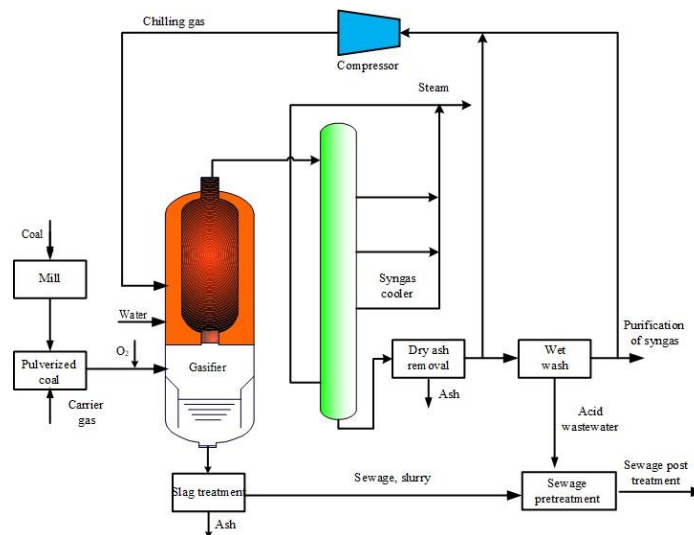


Figure 5. Schematic diagram of Shell gasifier

2.1.3 WGS

The crude gas produced by gasification unit mostly consists of H₂, CO, CO₂, H₂O (g), N₂, H₂S, COS, and CH₄. Before entering the F-T synthesis unit, the ratio should be adjusted to about 1.7 by water gas shift reaction. The water gas shift reaction is as presented in Eq. (1).



The hydrogen to carbon ratio is adjusted by a water shift reaction. The water shift reaction is assumed to reach chemical equilibrium. In this work, the crude gas of Lurgi gasifier can meet the requirement of the molar ratio of H₂ to CO. It is considered not essential for the WGS unit to be in the Lurgi CTL. The lowest molar ratio of H₂ to CO among the three processes is Shell CTL. According to the progress of the shift reaction, a two-stage shift reaction process was chosen in the Shell CTL process. The one-stage shift reaction process was applied in the Texaco CTL process.

For modelling the WGS unit, conversion reactor was simulated by an equilibrium reactor. SRK was chosen as the property method. The heat loads were set to 0 KW. The equilibrium temperature approach was used to adjust the reaction equilibrium. Details of the simulation refer to our previous work (Yang et al., 2017).

2.1.4 Rectisol unit

The Rectisol unit is a commonly used acid gas removal process. The process is a physical absorption gas purification method using low-temperature methanol as an absorbent. Low-temperature methanol has a relatively high solubility for acid gases such as H₂S, CO₂ in the raw synthesis gas, and can effectively remove the acidic gases in the raw synthesis gas. It ensures that the synthesis gas meets the requirement to obtain high-purity hydrogen in subsequently. The absorption tower absorbs the acid gas, and the desorption tower desorbs the acid gas and returns the lean methanol to the absorption tower to recycle the methanol.

For modelling the Rectisol unit, the absorption and desorption part were modelled

by RadFrac model. CPA, PSRK, and PC-SAFT were chosen as the primary property methods. The binary interaction parameters of PC-SAFT, PSRK, and CPA were regressed by the VLE data. The revised CPA, PSRK, and PC-SAFT methods were used for modelling the absorption tower, the desorption tower, and the rest, respectively. Details of the simulation could be found in the previous work (Yang et al., 2016).

2.1.5 *F-T synthesis unit*

To represent realistic installations of demo cases in China, a slurry bed was employed for F-T synthesis in this paper, where the Co-based catalyst was used. Slurry bed F-T synthesis reactors have been reported successful operation by Yankuang Group, Yiai Group, and Lu'an Group (Fox et al., 1995). The mole ratio of hydrogen to carbon requires to match 1.6-2.1. The slurry bed reactors have advantages on catalyst consumption and capital investment compared with fixed bed reactors.

The sulfur-free purified gas from the Rectisol unit is converted into hydrocarbon fuels. The synthesis reaction operates at 21 bar and 220 °C. The main mechanism of the F-T reaction is shown as Eq. (2).



where $\text{-CH}_2\text{-}$ represents the building block.

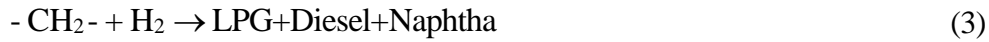
For modelling the F-T synthesis unit, RYield block was employed to model the synthesis reactor. Temperature and pressure were used as the specification parameters. The yields of heavy oil, diesel, and gasoline were set to 0.48, 0.19, and 0.19. The yields of synthetic fuels were confirmed to the previous research of Yates and Satterfield (1992).

2.1.6 *Hydrotreating and separation unit*

The hydrotreating and separation consist of unsaturated hydrocarbons and oxygenate hydrogenation; long-chain saturated hydrocarbons cracked into short-chain hydrocarbons to facilitate diesel production and oil separation.

The products of CTL are LPG, diesel, and naphtha. After F-T reactions, the

synthesis requires hydrotreating, which is shown in Eq. (3). Under the action of catalyst, the synthesis reacts with hydrogen gas to produce LPG, diesel, and naphtha.



The liquid fuels leaving the hydrotreating and separation unit is separated into LPG, diesel, and naphtha. For modelling hydrotreating and separation unit, Requil block was employed to model the reactions. The thermodynamic method is Peng-Rob equation of state. The composition of the fuels were calculated according to Ref (Zhou et al., 2016).

2.2 Flowsheet simulation

The flowsheet simulation of three different CTL processes is reported in this section (Aspen Tech, 2015). The feedstock is Lu'an coal. The lower heating value (LHV) of the feedstock is 29.82 MJ/kg. The ultimate analysis and proximate analysis are shown in Table 2. The basic parameters of each unit are presented in Table 3.

The feedstock conditions of the three processes are summarised in Table 4. The feedstock flowrates of Lurgi gasifier, Texaco gasifier, and Shell gasifier are 643 t/h, 502 t/h, and 429 t/h. The flow rates were determined for the production of the three processes, which match 1 million tons per year. Table 5 specifies the key parameters for the simulations of three different gasification processes.

Table 2. Ultimate analysis and proximate analysis of Lu'an coal

Proximate analysis (wt. %, ar)				Ultimate analysis (wt. %, ar)					
M ^a	FC ^b	V ^b	A ^b	ASH	S	N	O	H	C
1.2	72.3	11.6	16.0	16.0	0.2	1.0	4.7	3.4	74.7

a. Air dryness based.

b. Dryness based.

Table 3. The basic parameters of the units

Unit	Parameter	Value	unit	Parameter	Value
ASU	Power (kWh/t)	433	<i>F-T synthesis</i>	Reactor temperature (°C)	220

<i>Rectisol</i>	Lean temperature (°C)	-58	<i>Hydrotreating and Separation</i>	Pressure (bar)	21
	Absorber stage	35		CO conversion ratio	0.73
	Stage pressure drop (bar)	0.15		Pressure, bar	38

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Table 4. Feedstock for the three gasification processes

	Lurgi gasifier	Texaco gasifier	Shell gasifier
Coal (t/h)	643	502	429
O ₂ (Nm ³ /h)	210,333	308,582	308,997
Steam (t/h)	710	270	303

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Table 5. Specifications for simulating the three processes

Lurgi		Texaco		Shell	
<i>Gasification</i>		<i>Gasification</i>		<i>Gasification</i>	
Gasifier temperature (°C)	1,050	Gasifier temperature (°C)	1,280	Gasifier temperature (°C)	1,450
Oxygen to coal ratio	0.47	Oxygen to coal ratio	0.88	Oxygen to coal ratio	1.03
Steam to coal ratio	1.10	Steam to coal ratio	0.54	Steam to coal ratio	0.71
		<i>WGS</i>		<i>WGS</i>	
		Reaction temperature (°C)	280	Reaction temperature (°C)	280
		Pressure (bar)	38	Pressure (bar)	40
		Pressure drop (bar)	0.5	Pressure drop (bar)	0.7

1 Table 6. Industrial and simulation data comparison of the three processes

	Gasification				WGS				Rectisol		
	Fraction (mol%)	Simulation data	Industrial data	Error (%)	Simulation data	Industrial data	Error (%)	Simulation data	Industrial data	Error (%)	
Lurgi ^a	H ₂	39.94	41.41	3.55	-	-	-	55.11	54.92	-0.35	
	CO	26.51	24.23	-9.41	-	-	-	31.34	31.98	2.00	
	CO ₂	24.08	25.01	3.72	-	-	-	1.00	1.00	0.00	
	H ₂ S+COS	0.03	0.03	-	-	-	-	trace	trace	-	
	CH ₄	8.93	8.59	-	-	-	-	11.85	11.37	-	
	Others	0.51	0.67	-	-	-	-	0.7	0.68	-	
Texaco ^b	H ₂	34.01	35.71	4.76	42.78	43.4	1.43	60.08	60.46	0.63	
	CO	42.99	44.45	3.28	27.01	27.32	1.13	37.91	37.74	-0.45	
	CO ₂	21.02	18.98	-10.75	29.22	28.53	-2.42	1.00	1.45	-	
	H ₂ S+COS	0.4	0.31	-	0.3	0.27	-	trace	trace	-	
	CH ₄	0.13	0.09	-	0.1	0.08	-	0.15	0.11	-	
	Others	1.45	0.46	-	0.59	0.4	-	0.86	0.64	-	
Shell ^c	H ₂	32.91	32.28	-1.95	48.88	48.65	-0.47	66.31	66.16	-0.23	
	CO	65.12	65.73	0.93	25.81	25.67	-0.55	32.49	32.73	0.73	
	CO ₂	1.69	1.56	-8.33	25.02	25.35	1.30	1.00	0.87	-14.94	
	H ₂ S+COS	0.23	0.24	-	0.18	0.18	-	trace	0	-	
	CH ₄	0.03	0.02	-	0.02	0.02	-	0.1	0.1	-	
	Others	0.02	0.17	-	0.09	0.13	-	0.1	0.14	-	

2 a. Shanxi Lu'an CTL Ltd., 2008.

3 b. Shanxi Future Energy Ltd., 2015.

4 c. Shanxi Lu'an CTL Ltd., 2016.

5 Error (%) = (Industrial data-Simulation data)/ Industrial data*100%

The simulation results were compared with industrial data to ensure the reliability of the techno-economic analysis in the following section. It can be observed that simulation data of the main components show a good agreement with industrial data given in Table 6. The maximum error is the CO₂ content of purified gas out of the Rectisol unit, which is caused by the enthalpy calculation of the property method. Due to the few fraction of the component, it has nearly no influence on the techno-economic analysis of the three processes. The estimation is the basis for the techno-economic comparison of the three different gasifier processes discussed in later sections.

3. Three gasification methods comparisons

3.1 Energy efficiency

Energy efficiency is an important indicator to evaluate a process. Energy efficiency is the ratio of the produced and total energy (enthalpy based), which is shown as:

$$\eta = \frac{E_p}{E_T} \quad (4)$$

where E_p represents for the energy of the fuels which includes gasoline and diesel; E_T represents for the total energy consumption (chemical enthalpy) including raw material, steam and electricity.

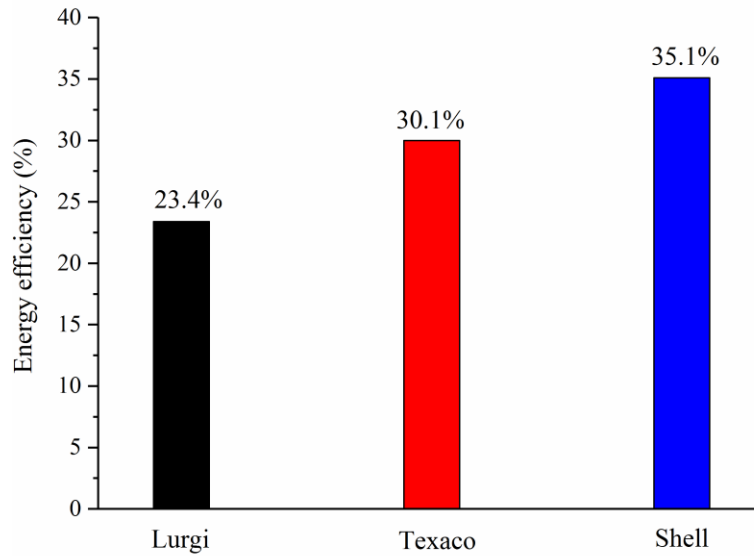


Figure. 6 Energy efficiencies of Lurgi, Texaco, and Shell CTL

The energy efficiency of Lurgi gasifier, Texaco gasifier, and Shell gasifier for CTL was calculated using Eq. (4). The results are shown in Fig 6. The energy efficiency of the Lurgi CTL is lower than Texaco CTL and Shell CTL. Shell CTL shows the best performance in terms of energy efficiency. The energy efficiency of Lurgi CTL, Texaco CTL, and Shell CTL is 23.4%, 30.1%, and 35.1%. Compared with Texaco CTL, the energy efficiency of Lurgi CTL is 77.7%, and Shell CTL is 116.6%. This implies that Lurgi CTL is 22.3% lower than Texaco CTL on energy efficiency, while Shell CTL is 16.6% higher. It is suggested to employ Shell CTL in the CTL process due to its high-energy efficiency, which reveals low GHG emissions.

3.2 Coal consumption

As the raw material of CTL is coal, coal consumption has a significant influence on the CTL process. In this section, an indicator of coal consumption is used to analyse the performance of CTL. Coal consumption is defined as the ratio of coal to fuel, which can be calculated by:

$$\varphi_{cc} = \frac{m_c}{m_p} \quad (5)$$

where m_p represents for the weight of the fuels, which includes the weight of gasoline and diesel; m_c represents for the weight of coal.

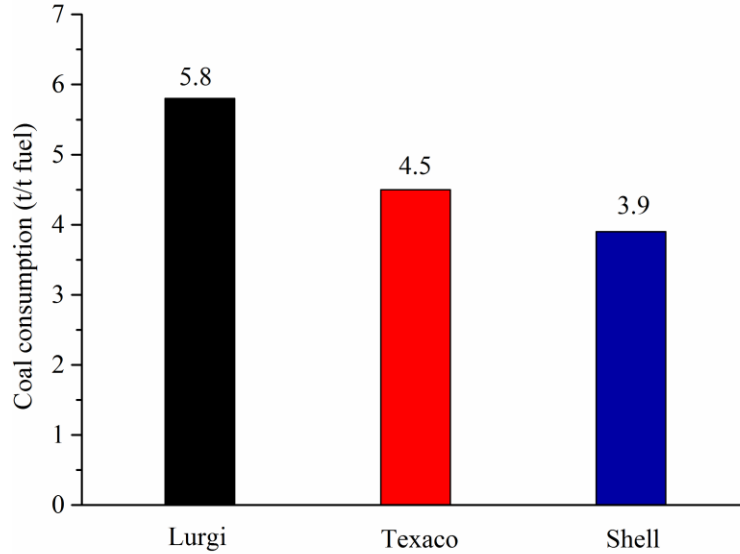


Figure. 7 Coal consumption of Lurgi, Texaco, and Shell CTL

The coal consumption of Lurgi, Texaco, and Shell CTL was calculated based on Eq. (5) and shown in Fig 7. The coal consumptions of Lurgi, Texaco, and Shell CTL are 5.8 t/t, 4.5 t/t, and 3.9 t/t fuel. Shell CTL shows the best performance with the lowest coal consumption. It suggests that the Shell CTL consumes the lowest coal per unit fuel. When compared to Texaco CTL, the coal consumption of Lurgi CTL is 128.9%, and Shell CTL is 86.7%. It implies that Lurgi CTL is consuming 28.9% more than Texaco CTL, while Shell CTL consumes 13.3% less. For this reason, for the CTL process, it is suggested to employ Shell CTL considering its low coal consumption.

3.3 Utility consumption

Utility consumption is also an vital evaluation indicator for the CTL process. The utilities for CTL include water, electricity, and steam. Water consumption, electricity consumption, and steam consumption of Lurgi, Texaco, and Shell CTL are discussed in this section.

3.3.1 Water consumption

Water consumption is defined as the ratio between the weight of water consumed in CTL and the weight of the fuel, which is formulated as follows:

$$\varphi_{wc} = \frac{m_w}{m_p} \quad (1)$$

where m_w is the weight of water consumed in the whole CTL process.

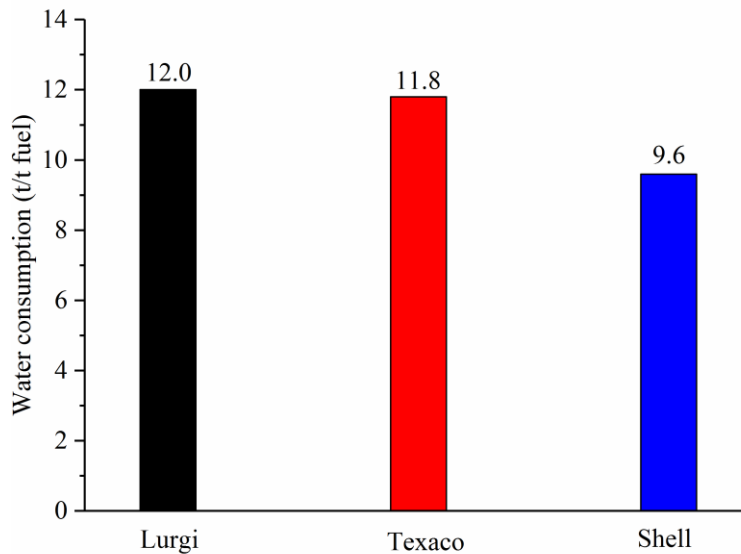


Figure. 8 Water consumption of Lurgi, Texaco, and Shell CTL

The main process of the CTL with different gasifiers is the CG. The results of the water consumption are presented in Fig. 8. The water consumption of Lurgi CTL process is the highest. The Texaco CTL process has no significant difference in water consumption with Lurgi CTL, and the Shell CTL is the lowest. The water consumption of

Lurgi is 12.0 t/t, Texaco 11.8 t/t, and Shell CTL 9.6 t/t of fuel. The water consumption of shell CTL is 80.0% of that of Lurgi CTL, and 81.3% in that of Texaco CTL. It can be obtained that Shell gasifier is the best choice for the CTL process in water-deficient areas.

3.3.2 Oxygen consumption

Oxygen consumption indicates the size of ASU, which affects the capital cost, steam consumption, etc. Oxygen consumption is the proportion of oxygen standard volume to the weight of the fuel, which can be formulated as Eq. (7).

$$\varphi_{oc} = \frac{V_o}{m_p} \quad (2)$$

where V_o represents the standard volume of consumed oxygen in the whole process of CTL.

The oxygen consumption of Lurgi, Texaco, and Shell CTL is calculated based on Eq. (7) and the results are shown in Fig 9. The Lurgi CTL has the lowest oxygen consumption, and the Shell CTL has the highest. The oxygen consumption of Lurgi, Texaco, and Shell CTL is 1,123, 2,109, and 2,497 Nm³ per t fuel. When compared to Texaco CTL, the oxygen consumption of Lurgi CTL is 53.2%, and Shell CTL is 118.4%. This implies that Lurgi CTL is 46.8% lower than Texaco CTL on oxygen consumption, while Shell CTL is 18.4% higher. It can be observed that the Lurgi CTL exceeds in terms of oxygen consumption compared to Texaco CTL and Shell CTL.

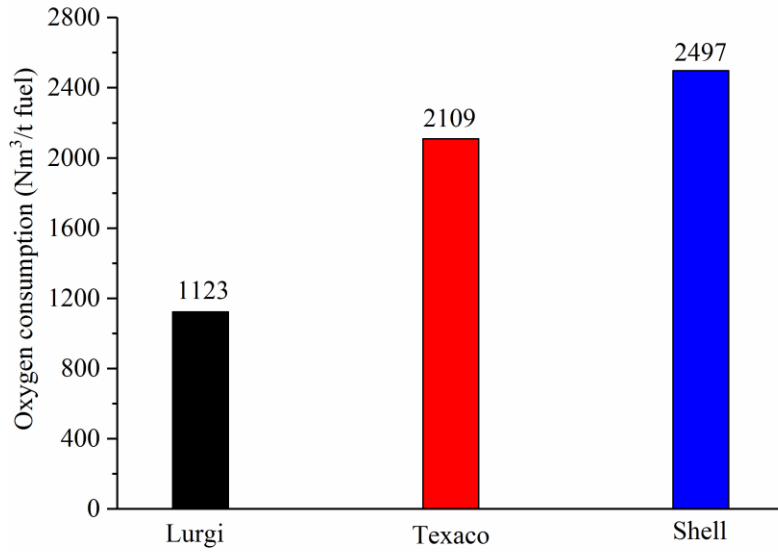


Figure. 9 Oxygen consumption of Lurgi, Texaco, and Shell CTL

3.3.3 Steam consumption

The steam consumption is defined as the ratio between the energy of consumed steam and the weight of the fuel, which can be expressed as Eq. (8).

$$\varphi_{sc} = \frac{E_s}{m_p} \quad (3)$$

where E_s represents the energy of all steam at all levels consumed in the whole process of CTL.

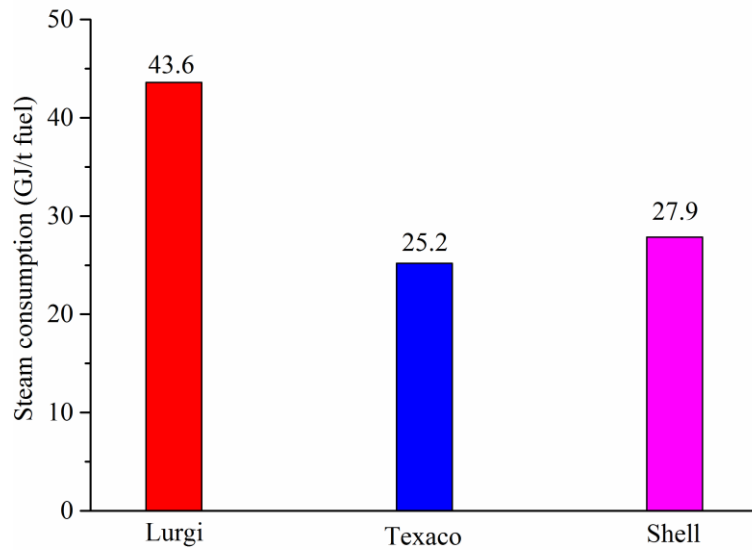


Figure. 10 Steam consumption of Lurgi, Texaco, and Shell CTL

The steam consumption of Lurgi, Texaco, and Shell CTL is calculated based on Eq (8), and the results are shown in Fig 10. The steam consumption of Lurgi CTL, Texaco CTL, and Shell CTL are 43.6, 25.2, and 27.9 GJ/t fuel. Texaco CTL has the lowest value of steam consumption, which is 57.8% of that in Lurgi CTL and 90.3% of Shell CTL. On the view of steam consumption, Texaco CTL is the best choice for CTL. Typically, steam is generated from fuel coal in a coal-based plant. In the abundant coal area, there is no significant difference between the Texaco gasifier and Shell gasifier for CTL in terms of steam consumption.

3.4 Total capital investment

Total capital investment includes fixed capital investment and working capital investment. Fixed capital investment is purchasing plant facilities, and working capital investment is maintaining the plant operation. The equipment investments of CTL process are calculated by Eq. (9).

$$I_2 = I_1 \left(\frac{Q_2}{Q_1} \right)^{sf} \quad (4)$$

where I_1 represents the reference equipment investment; Q_1 represents the reference project scale; I_2 represents the studied equipment investment; Q_2 represents the studied project scale; sf represents the exponent (0.6 in this paper) (Zhou et al., 2016).

Table 7. Capital investment ratio factors

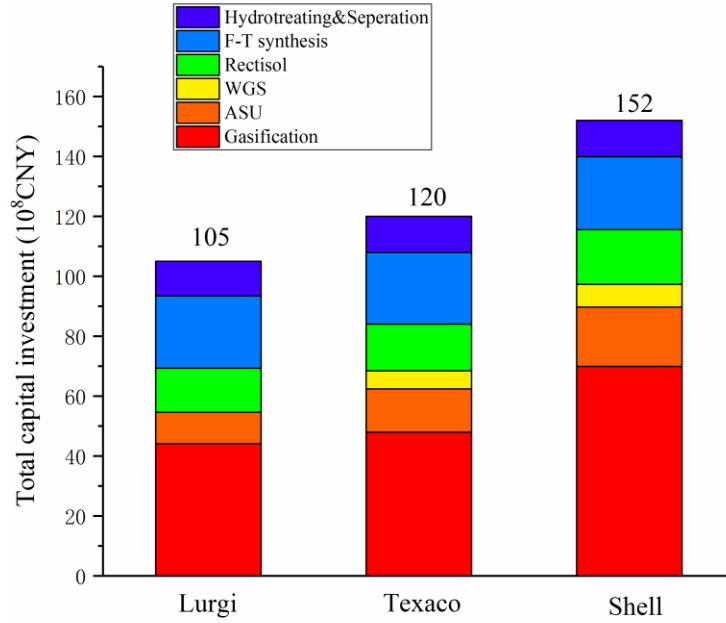
Component	Ratio factor, RF (%)
(1) Direct investment	181
(1.1) Buildings (including services)	25
(1.2) Land	6
(1.3) Electrical	10
(1.4) Instrumentation and controls	15
(1.5) Piping	15
(1.6) Installation	10
(1.7) Equipment	100
(2) Indirect investment	75
(2.1) Contingency	15
(2.2) Contractors fees	20
(2.3) Construction	25
(2.4) Engineering and supervision	15
(3) Fixed capital	256
(4) Working capital	50
(5) Total capital	306

Values of the equipment investment and the reference systems scale are collected from the literature. The Gasification, ASU, WGS, and Rectisol units are referred to Yang et al. (2017) and Xiang et al. (2014). The F-T synthesis and Hydrotreating& Separation units are referred to (2011) and later Zhou et al. (2016). The equipment investment of the

119 CTL processes was calculated by Eq. (9). Other fixed investments are calculated by
120 equipment investment multiplied by corresponding factors, which are shown in Table 7.
121 The total investment of the CTL processes can be calculated as follows:

$$TCI = EI(1 + \sum RF_i) \quad (5)$$

where TCI represents total capital investment; EI represents equipment investment;
 i represents the components of the investment, and RF represents the ratio factor.



125125

126 Figure. 11 Total capital investments and investments compositions of Lurgi, Texaco, and Shell CTL

127127

128 As depicted in Fig. 11, the total capital cost of Lurgi, Texaco, and Shell CTL is
 129 calculated by Eq. (10). The total capital cost of Lurgi CTL is 105×10^8 CNY; the cost of
 130 Texaco CTL is 120×10^8 CNY; the Shell CTL is 152×10^8 CNY. The total capital
 131 investment of Lurgi CTL is 69.1% of that Shell CTL and 87.5% of Texaco CTL. It can be
 132 obtained that Lurgi gasifier is recommended for CTL due to its minimal total capital cost.

133 The total capital investment of Texaco and Shell CTL are divided into six
 134 subsystems (Lurgi CTL is five subsystems). The investment compositions are presented
 135 in Fig 8. The compositions show that the coal gasification unit constitutes the most
 136 significant part, accounting for 42% of the total capital investment for Lurgi CTL, 40%
 137 for Texaco CTL, and 46% for Shell CTL. F-T synthesis and Rectisol unit also have

remarkable contributions, occupying 23% and 14% in Lurgi CTL, 20% and 13% in Texaco CTL, and 16% and 12% in Shell CTL. The proposed investments of the subsystems not only depend on their material requirements and installation complexity but also are strongly associated with their current degree of development in China. It is advised that the gasification unit should be focused on the development of gasifier technology. Additionally, F-T synthesis and Rectisol technology are also contributing significantly to CTL development. Lurgi gasifier is suitable for CTL process in pilot demonstration projects for the low investment.

3.5 Production cost

Production Cost (PC) mainly includes utility, raw material, and others cost. PC is calculated using Eq. (11):

$$PC = C_R + C_U + C_{O\&M} + C_D + C_{POC} + C_{AC} + C_{DSC} \quad (6)$$

where C_R is raw material cost; C_U is utility cost; $C_{O\&M}$ is operating and maintenance cost; C_D is depreciation cost; C_{POC} is plant overhead cost; C_{AC} is administrative cost; C_{DSC} is distribution and selling cost.

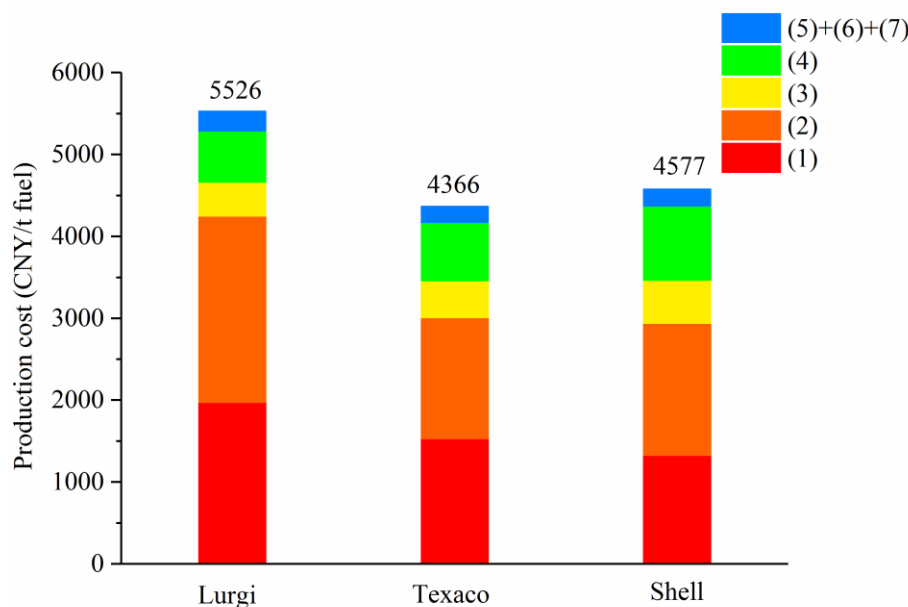
Table 8. Production cost calculation assumptions

Component	Economic assumption
(1) C_R	Coal 340 CNY/t (Khosrow et al., 2015)
(2) C_U	Electricity 0.5 CNY/kWh (Yang et al., 2016); Steam 42 CNY/GJ (Xiang et al., 2014); H ₂ O 2 CNY/t (Yang et al., 2018)
(3) $C_{O\&M}$	
(3.1) Operating workers	100,000 CNY/person/y; 1,500 workers
(3.2) Direct supervisory & clerical labour	10 % of operating labour
(3.3) Maintenance and repairs	2 % of fixed capital investment
(3.4) Operating supplies	0.7 % of fixed capital investment
(3.5) Laboratory charge	10 % of operating labour
(4) C_D	Salvage value 4%; Life period 15 y
(5) C_{POC}	5% (3.1+3.2+3.3)
(6) C_{AC}	2% of PC

(7) C_{DSC}	2% of PC
(8) PC	(1) + (2) + (3) + (4) + (5) + (6) + (7)

155155

156 Some assumptions are shown in Table 8. The depreciation cost is calculated by a
157 straight-line method. The production costs of these processes were calculated based on
158 Eq. (11). A further breakdown of the results is shown in Fig. 12. It can be obtained that
159 the production costs of Lurgi are 5,526, Texaco 4,366, and Shell CTL 4,577 CNY/t fuel.
160 The production cost of Texaco and Shell CTL is similar and lower than that of Lurgi
161 CTL.



162

163 Figure. 12 Production costs of Lurgi, Texaco, and Shell CTL

164 For Lurgi CTL, the largest production cost is utility cost, accounting for 41.2% of the
165 total production cost. Raw material cost and depreciation cost are accounting for 35.7%
166 and 11.3%. The optimisation of utility network can improve the Lurgi CTL energy
167 efficiency and economy. Raw material cost, utility cost, and depreciation cost account for
168 35.0%, 33.9%, and 16.4% in Texaco CTL. In Shell CTL, raw material cost, utility cost,
169 and depreciation cost are 25.6%, 35.3%, and 19.8%. The difference between the Texaco
170 CTL and the Shell CTL is large due to the depreciation cost. This is explained by the fact

that the total capital cost of Shell CTL is 1.27 times that Texaco CTL. It is recommended to using Texaco gasifier for CTL process in terms of production cost.

3.6 CO₂ emission

GHG emission is a significant environmental parameter (Čuček et al., 2015). In this section, GHG emission is defined as the ratio of CO₂ emissions in CTL to the production of CTL (which includes LPG, diesel, and naphtha) as shown in Eq. (12). The CO₂ emissions in CTL is mainly from the tail gas in Rectisol and F-T synthesis units.

$$E_{CO_2} = \frac{m_{CO_2}}{m_{LPG} + m_{Diesel} + m_{Naphtha}} \quad (12)$$

where m_{CO_2} represents the annual carbon emission in CTL; m_{LPG} represents the annual production of LPG in CTL (t/y); m_{Diesel} represents the annual production of diesel in CTL (t/y); $m_{Naphtha}$ represents the annual production of naphtha in CTL (t/y).

Fig 13 shows the GHG emissions of Lurgi, Texaco, and Shell CTL. The GHG emissions of Lurgi, Texaco, and Shell CTL are 5.26 t/t fuel, 4.86 t/t fuel, and 3.49 t/t fuel. The ratios of the CO₂ in Rectisol and F-T synthesis units are different in Lurgi, Texaco, and Shell CTL due to the different carbon-hydrogen ratio in raw crude gas and purified gas, which significantly affects the reactions in both units. The CO₂ emission ratio of Rectisol is 97.1% in Lurgi CTL because of the highest carbon-hydrogen ratio, followed by Shell CTL, accounting for 89.1%. The CO₂ emission ratio of Rectisol in Texaco CTL is the lowest, which is 87.0%. It suggests that the Shell CTL consumes the lowest CO₂ emission per unit fuel. When compared to Shell CTL, the GHG emission of Lurgi CTL is 150.7%, and Texaco CTL is 139.2%. It implies that Lurgi CTL emits 50.7% CO₂ more than Shell CTL, and Texaco CTL emits 39.2% more. Consequently for the CTL process, it is suggested to employ Shell CTL in the view of GHG emission.

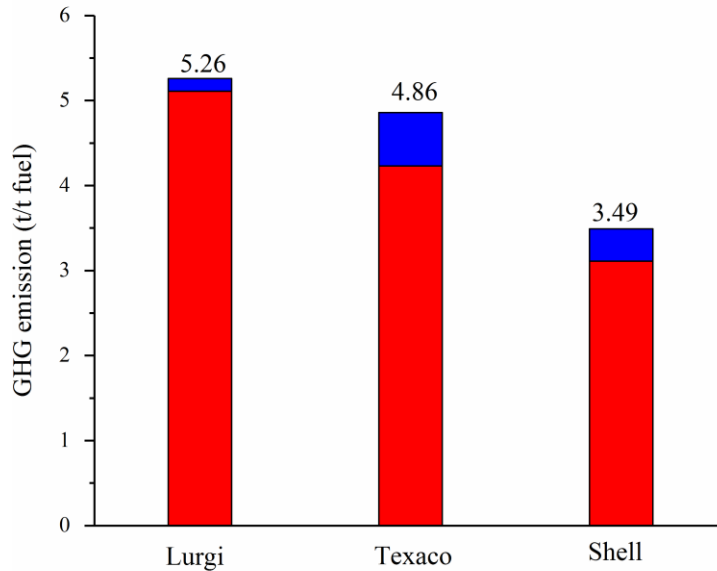


Figure. 13 GHG emissions of Lurgi, Texaco, and Shell CTL

3.7 Influences of coal price on fuel production cost

The production cost is significantly influenced by coal price. In this section, the coal price is analysed. The production costs of the three processes were calculated based on Eq. (11). The simulation results are shown in Fig. 14. The abscissa is coal price, which varies from 100 CNY/t to 800 CNY/t. The ordinate represents production cost.

With the increase in coal price, the production cost increases. The production cost of Lurgi CTL is more expensive than that of Texaco CTL and Shell CTL. Further increase in the coal price, the gap between the production cost of Lurgi CTL with the production costs of Texaco CTL and Shell CTL is increasing. The Texaco CTL shows a better performance than Shell CTL on production cost at a low coal price. The increase in coal price decreases the gap between the production costs of Texaco CTL and Shell CTL. With the increase of coal price, the production cost of Texaco CTL equals to that of Shell CTL at a coal price of 677 CNY/t. It can be concluded that Lurgi CTL is not suited for

large-scale commercial production. Shell CTL exhibits a better performance on resistance to high coal price compared with Lurgi CTL and Texaco CTL.

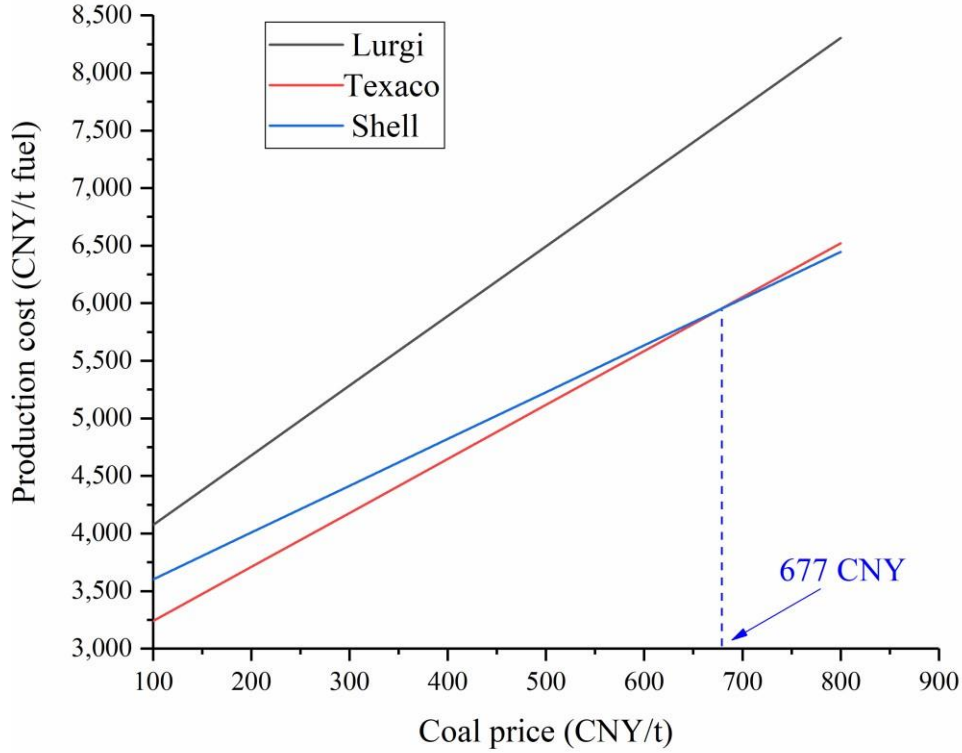


Figure. 14 Coal price analysis of Lurgi, Texaco, and Shell CTL

3.8 Carbon tax

The aim of a carbon tax is greenhouse gas effects reduction and environment protection. A carbon tax is analysed in this section. The performances of Lurgi CTL, Texaco CTL, and Shell CTL were evaluated by production cost. The production cost considering carbon tax is calculated as follows (Yang et al., 2018):

$$PC_{carbon-tax} = PC + f_{carbon-emission} \times CT \quad (13)$$

where $PC_{carbon-tax}$ represents the production cost considering carbon tax; PC represents the production cost which discussed in the earlier section; $f_{Carbon-emission}$

221 represents the carbon emission; CT represents carbon tax.

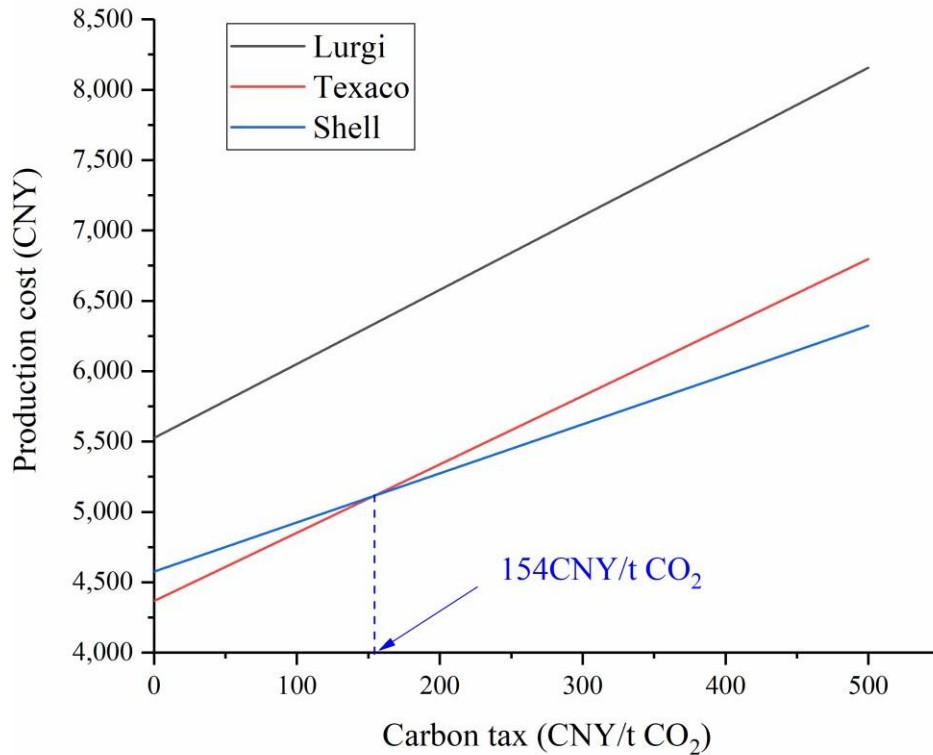


Figure. 15 Carbon tax analysis of Lurgi, Texaco, and Shell CTL

The production costs (considering carbon tax) of Lurgi CTL, Texaco CTL, and Shell CTL were calculated by Eq. (13) and are shown in Fig. 15. The production cost of the three processes increases with the increase in carbon tax. The production cost of Lurgi CTL is more expensive than that of Texaco CTL and Shell CTL regardless of considering carbon tax or not. The production cost of Texaco CTL is lower than that of Shell CTL at a cheap carbon tax. The difference in the production cost of Texaco CTL and Shell CTL is reduced as the increase of carbon tax. A further increase, the production cost of Texaco CTL equals to that of Shell CTL at 154 CNY/t carbon tax. While increasing the carbon tax, the Shell CTL shows a better performance. It can be concluded that Texaco CTL shows the best performance at a low carbon tax and Shell CTL has the best performance

when the carbon tax is expensive than 154 CNY/t. Shell CTL can well adapt to carbon tax policy.

4. Conclusions and prospects

This paper aims to provide suggestions for the cleaner production and sustainable development of CTL technology. Lurgi CTL, Texaco CTL, and Shell CTL were extensively modelled and simulated. Techno-economic analysis of the three gasification processes was conducted based on the calculation results. The conclusions can be summarised as below:

1. The energy efficiency of Lurgi CTL is 23.4%, Texaco CTL 30.1%, and Shell CTL 35.1%. This is mainly decided by the consumptions of coal and utilities in the CTL with different gasifiers. The coal consumptions of Lurgi are 5.8 t/t fuel, Texaco 4.5 t/t fuel, and Shell CTL 3.9 t/t fuel, and the utilities of these three gasifiers are 43.6 GJ/t fuel, 25.2 GJ/t fuel, and 27.9 GJ/t fuel. The consumption of coal and utilities of Texaco and Shell processes are much lower than that of the Lurgi process, therefore Texaco gasifier interconnected with Lurgi gasifier or Shell gasifier interconnected with Lurgi gasifier will reduce the consumption of coal and utilities of single Lurgi process and then reduce CO₂ emission to a great extent, and also increase the whole energy efficiency of the integrated CTL.
2. The total capital cost of Lurgi CTL is 105×10^8 CNY; the cost of Texaco CTL is 120×10^8 CNY; the Shell CTL is 152×10^8 CNY. The coal gasification unit accounts for 42% of the total capital investment for Lurgi CTL, 40% for Texaco CTL, and 46% for Shell CTL. Gasification unit occupies the most significant proportion of total capital investment of CTL processes. Coal gasification technology may be potentially limiting the overall acceptance and practice of CTL in the future. Developing novel gasification technology to reduce the cost would definitely be of high interest to the industry. The production costs of Lurgi, Texaco, and Shell CTL are 5,526, 4,366, and 4,577 CNY/t fuel. The GHG

emissions of Lurgi, Texaco, and Shell CTL are 5.26 t/t fuel, 4.86 t/t fuel, and 3.49 t/t fuel. It is suggested to employ Shell CTL in the view of GHG emission. The coal accounts for 35.7% of the production cost for Lurgi CTL, 35.0% for Texaco CTL, and 25.6% for Shell CTL. Shell CTL exhibits a better performance on resistance to high coal price compared with Lurgi CTL and Texaco CTL. Additionally, Lurgi gasifier has much lower capital investment while Texaco gasifier and Shell gasifier have much lower production cost. From economic point of view, Texaco gasifier interconnected with Lurgi gasifier or Shell gasifier interconnected with Lurgi gasifier will realize the trade-off between capital investment and production cost when compared with single gasifier.

3. Shell gasifier is potentially the best option for the CTL process in the water-deficient area, for example, Xinjiang province. Texaco gasifier is a potential alternative for the CTL process where coal and water resource are abundant, for example, Anhui province. Lurgi gasifier is suitable for CTL process in pilot demonstration projects. In addition, Shell gasifier is recommended for a region without visible defects due to low GHG emission, for example, Shandong province.

Different alternatives interconnected may have the potential to promote the development of CTL. There are three interconnected possibilities: Shell gasifier interconnected with Texaco gasifier, Shell gasifier interconnected with Lurgi gasifier, and Lurgi gasifier interconnected with Texaco gasifier. Shell gasifier and Texaco gasifier have less promotion on coal consumption, water consumption, or others. Combining the results of this context with our previous research, conclusions can be obtained. Shell gasifier and Lurgi gasifier can be interconnected with coal consumption because the different alternatives consume the coal on different particle size. Lurgi gasifier would produce a large amount of wastewater, which is challenging to be treated. This would reduce the performance of Lurgi gasifier. Whereas, the wastewater can be used in Texaco gasifier to

288 reduce water consumption in Texaco CTL. Lurgi gasifier and Texaco gasifier can be
289 interconnected to cut down water consumption. Our future work will focus on
290 quantifying the reduced consumption by the interconnection.

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297 **Notes**

298 The authors declare no competing financial interest.

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300 **Acknowledgements**

301 The authors would like to thank the financial support from the China NSF project

304 (NO. 51676209 and 51606224).

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