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Techno-economic analysis and comparison of coal-based chemical technologies with consideration of water resources scarcity

Jinyang Zhao [a], Li Zhou [b], Wenji Zhou [c], Hongtao Ren [a], Yadong Yu [a,*], Fuchen Wang [d], Tieju Ma [a,e,**]

[a] School of Business, East China University of Science and Technology, Shanghai, 200237, China
[b] Institute of Energy, Environment and Economy, Tsinghua University, Beijing, 100084, China
[c] School of Applied Economics, Renmin University of China, Beijing, 100872, China
[d] Institute of Clean Coal Technology, East China University of Science and Technology, Shanghai, 200237, China
[e] International Institute for Applied Systems Analysis (IIASA), Laxenburg, Austria

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ABSTRACT

Existing techno-economic analyses of modern coal chemical technologies (MCCTs) neglect water constraints, which may underestimate the production cost of MCCTs and thus mislead investment activities. Considering this background, this study incorporated water scarcity and indirect water cost into a classic techno-economic evaluation model of MCCT. Using this model, our work evaluated and compared the techno-economic indicators with the latest data for four typical MCCTs, including coal-to-liquids (CTL), synthetic natural gas (SNG), coal-to-olefin (CTO), and coal-to-ethylene glycol (CTEG). The results demonstrate the following: 1) The production costs of CTL, SNG, CTO, and CTEG are 5185 CNY/t, 2653 CNY/kNm^3, 5918 CNY/t, 4055 CNY/t, respectively. Under the current prices of oil-related products, investment in SNG and CTEG would be risky, investment in CTL should be considered cautiously, and investment in CTO could lead to a profit. 2) Under the current market price of water resources, which does not consider the water constraint of MCCTs, the production cost would be underestimated by at most 12.4% for CTL, 10.6% for SNG, 27.5% for CTO, and 32.4% for CTEG. The sensitivity of the results to some key parameters and investment recommendations considering profitability, capital investment, material consumption, water constraints, and CO_2 emissions are also discussed and provided.

1. Introduction

In 2018, China imported more than 461 million tons of oil, which accounted for 72% of China's total oil consumption [1]. Because of low oil reserves in China [2], its dependence on oil imports will continue to increase in the future, which will significantly challenge China's energy security [3]. Therefore, developing alternative technologies to produce oil products is important, e.g., developing modern coal chemical technology (MCCT) to produce oil from coal, which is a relatively abundant resource in China [4]. In comparison with traditional coal chemical technology, which is a byproduct of the steel industry, MCCT uses coal to produce syngas, liquid fuels, olefins, and other petrochemical substitutes [5]. Here, the considered technologies in MCCT include coal-to-liquids (CTL), coal-to-olefins (CTO), synthetic natural gas (SNG), and coal to ethylene glycol (CTEG) [5]. In recent years, MCCT has attracted the interest of the Chinese government; thus, it has undergone rapid development. Using CTL as an example, the production capacity for CTL reached 9.73 million t/y at the end of 2020 and was predicted to be 18.1–29.4 million t/y by 2030 [6].

Despite rapid development, water constraints and profitability concerns make MCCT highly controversial for policy-makers [7]. Water consumption is very high for all MCCTs. For example, according to the estimates of Guo et al. and Xiang et al. the direct water consumption amounts for 1 t of liquid fuel and olefin are 5.6 t and 30 t, respectively [7,8]. In general, to reduce coal transportation cost, coal chemical plants are frequently located in places rich in coal resources [7]. However, most coal-rich places in China, such as Inner magnolia, Ningxia, and Xinjiang, lack water [8]. The reverse distribution between water and coal has challenged the further development of MCCT. In addition to the water constraint, the profitability of MCCT, which is determined by coal

* Corresponding author.
** Corresponding author. School of Business, East China University of Science and Technology, Shanghai, 200237, China.
E-mail addresses: yuyd@ecust.edu.cn (Y. Yu), tjma@ecust.edu.cn (T. Ma).

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and oil prices and the technology investment cost [9], also poses a challenge to the application of MCCTs. Therefore, evaluating the techno-economic performance of MCCTs by considering water constraints should be conducted to further promote their development.

In the existing literature, the techno-economic performance of MCCT has been studied for many technologies, such as CTL [10–16], CTO [9, 17–21], SNG [14,22–24], and CTEG [25,26]. Such studies are summarized in Table 1. These papers provide primary data on certain technologies that may be beneficial for investment in MCCT. However, recent studies frequently used market prices to calculate the water cost of technologies while seldom considering water scarcity. For example, Xiang et al. [9,19–21] conducted detailed techno-economic evaluations and environmental impacts of CTO and coal-based Fischer--Tropsch-to-olefins (CFTO) plants with carbon capture and sequestration under the market prices of coal and water. Moreover, they only considered the direct water cost while neglecting the indirect water cost, e.g., the cost from wastewater treatment or water infrastructure construction [19,26]. This may result in the underestimation of the potential production cost of these technologies and mislead investors.

In addition, current research primarily focuses on the techno-economic evaluation of individual MCCTs while seldom comparing the techno-economic performance of different MCCTs. This type of study is important because it can aid potential stakeholders in selecting their investment direction by providing more comprehensive technical information, such as profit, cost, and risk.

In recent years, the relevant data (e.g., cost) of certain technologies have changed significantly, primarily because of the changes in prices of raw materials, labor cost, and domestic technological breakthroughs. For example, the largest single coal chemical project approved by China's National Development and Reform Commission during the "13th Five-Year Plan" period with a total investment of more than 120 billion CNY, namely, the 400,000 t/year ethylene glycol project of Yulin Energizing, is based on the "coal-based syngas catalytic synthesis of ethylene glycol technology," which is a technology process developed independently by Chinese University and the company, with full independent intellectual property rights. However, these latest data have not been reflected in current research, which may also mislead investors.

Therefore, this paper incorporates water scarcity and indirect water cost in a classic techno-economic evaluation model of MCCT. Using this model, this paper evaluates and compares the techno-economic indicators with the latest data for four typical MCCTs, including CTL, SNG, CTO, and CTEG. A brief introduction of selected technologies is provided in Section 2.1, while detailed process descriptions, key operation condition parameters and commercialized projects of these MCCTSs in China are provided in the **Supporting Information (SI)**. The remainder of this paper is structured as follows. Section 2 introduces the method and data used in this study. Section 3 presents the preliminary results, and Section 4 discusses the sensitivity of the results. Section 5 provides investment recommendations and policy suggestions. Section 6 concludes this paper.

Table 1
Summary of techno-economic performances and economic assumptions of MCCTs in the existing literature.

Technology	Production capacity	Total capital investment (Billion CNY)	Coal price	Production cost (CNY)	Data sources
CTL	2.0 Mt/y	37.0	50	4143	[10] [a]
	3.0 Mt/y	35.4	600	3811	[11]
	1.0 Mt/y	12.0	340	4293	[12]
	3.0 Mt/y	30.0	660	5013	[13]
CTO	0.7 Mt/y	17.6	640	6400	[17]
	0.7 Mt/y	17.6	640	6300	[18]
	0.7 Mt/y	20.7	620	7131	[19]
SNG	4.0 bm^3/y	27.3	160	2.2	[22]
	02 mm^3/y	5.7	658	2.52	[14]
CTEG	0.3 Mt/y	5.1	400	4663	[25] [b]
	0.3 Mt/y	5.1	400	4606	[26]

[a] The total capital investment and production cost in the literature with the unit of Canadian dollar is converted into CNY according to the exchange rate of 5.

[b] The total capital investment and production cost in the literature in units of US dollars are converted into CNY according to the exchange rate of 7.

2. Method and data

2.1. Technology introduction

In this work, four mainstream commercialized MCCTs, namely, CTL, SNG, CTO and CTEG, were selected for study because of their technological process similarities. They all start with air separation and coal gasification. After cooling, adjustment of the hydrocarbon ratio and purification, the crude syngas is converted into pure syngas and fed into further reactions, and the differences in subsequent reactions distinguish these four technologies from each other. More information about these technologies can be found in the **SI.**

- CTL: Pure syngas is sent into a Fisher-Tropsch (F-T) synthesis reactor to produce liquid fuel, including gasoline diesel and wax. After hydrocracking, the products are upgraded, and the diesel and gasoline are separated.
- SNG: Pure syngas is sent into the methanation reaction reactor to produce methane. After compression and dying in the following reactor, compressed natural gas is produced.
- CTO: Pure syngas is sent in a methanol synthesis unit to produce methanol. Then, methanol is used to produce ethylene and propylene in methanol to olefin units.
- CTEG: Pure syngas is used to synthesize dimethyl oxalate (DMOS) in the DMOS unit, and then DMOS is used as an intermediate to produce ethylene glycol (EG) in the EG synthesis unit. Finally, after processing in the refining unit, pure EG is produced.

2.2. Techno-economic evaluation model

In this study, a classical techno-economic evaluation model and economic indicators that are widely used in the assessment of chemical engineering technologies [27–32] were employed to evaluate the performance of different MCCTs. These indicators include total capital investment (TCI), production cost (PC), net present value (NPV), return on investment (ROI), and payback period (PP).

2.2.1. Total capital investment

The TCI is the sum of fixed capital investment, which is used to purchase and install equipment, and working capital investment, which is the required cost to maintain the function of the plant [9]. In this study, the TCI was calculated based on a coefficient approach [33], which is shown in Eq. (1).

$$TCI = EI \times \left(1 + \sum_i RF_i\right) \tag{1}$$

where EI is the equipment investment (e.g., air separation unit, coal gasification unit), and RF_i is the ratio factor of capital investment of component i to EI, including piping line, electricity, and land. As Eq. (2) shows, EI is the sum of all individual equipment investments (EI_j).

$$EI = \sum_j EI_j \tag{2}$$

Individual equipment investment can be calculated using a scaling-up approach [33]. Following most of the studies in the literature, this study also used the production capacity indicator to scale-up EI (Eq. (3)).

$$EI_j = \theta_j \times EIr_j \times \left(\frac{S_j}{Sr_j}\right)^{\alpha_j} \tag{3}$$

where EI_j is the equipment investment at production capacity S_j for equipment j, EIr_j is the equipment investment at the reference production capacity Sr_j, θ_j is the domestic element, and α_j is the scale index. The values of parameters (RF_i, θ_j, and α_j) and the benchmark scale of equipment investment (Sr_j and EIr_j) are shown in Tables 2 and 3.

Considering the time value of the investment, the relationship between the historical value and the current value of *TCI* is reflected by Eq. (4):

$$TCI_t = TCI_{t0} \times (1+\delta)^{t-t0} \tag{4}$$

where TCI_t and TCI_{t0} are the total capital investment at any given time t and base year $t0$, respectively, and δ is the average discount rate [22].

2.2.2. Production cost

PC is another important indicator of the economic performance of MCCT and can be calculated using Eq. (5) [9]. The PC consists of two parts: fixed operating and maintenance costs (C_{Fom}) and variable operating and maintenance costs (C_{Vom}) [13].

$$PC = C_{Vom} + C_{Fom} \tag{5}$$

C_{Vom} is the cost that changes with the change in production amount and can be calculated using Eqs. (6)–(8). It consists of two parts: C_r, which is the cost of raw material, andC_u, which is the cost of utilities such as water and electricity.

$$C_{Vom} = C_r + C_u \tag{6}$$

$$C_r = Q_r \times P_r \tag{7}$$

$$C_u = \sum_l Q_l \times P_l \tag{8}$$

The raw material cost (C_r) and utility cost (C_u) were calculated based on the material consumption amount and the latest corresponding market price. The raw material consumption of different technologies was obtained from the process simulation results in the existing literature. Detailed data are summarized and presented in Table 4. In Eqs. (7) and (8), Q_r and Q_l are the consumption amount of the raw material and utilities, respectively, and P_r and P_l are the latest market prices of the corresponding raw materials and utilities.

In contrast, C_{Fom} is the cost that does not change with the change in production amount, including the operation and maintenance cost ($C_{o\&m}$), cost of administration (Cad), and the cost of selling and distribution cost ($C_{S\&d}$). It is worth notice that *TCI* is also involved in the C_{Fom} as the form of cost of depreciation (C_d). And all these parameters can be calculated using Eqs. (9)–(19).

Table 2
Ratio factors of capital investment.

Component	CTL	SNG	CTO	CTEG
(1) Direct Investment	100	100	100	100
(1.1) Equipment	51	54	46	53
(1.2) Main installing materials	23	20	24	20
(1.3) Installation	12	12	13	12
(1.4) Construction	14	14	17	15
(2) Indirect investment	21	20	20	19
(2.1) Engineering and supervision	13	12	12	11
(2.2) Unforeseen fees	8	8	8	8
(3) Land	3	3	3	3
1 Fixed capital (1) +(2) +(3)	124	123	123	122
2 Intangible assets	3	3	4	3
3 Deferred assets	3	2	2	2
4 Financing cost	8	8	8	7
5 Working capital	5	5	4	4
Total capital 1 + 2+3 + 4	143	141	141	138

Table 3
Benchmarks for equipment investment.

Unit	Benchmark	α_j	θ_j	s_{rj}	$EI_{r,j}$(10^8 CNY)
Front-end technology[a,b]					
Coal handling	Daily coal input	0.67	0.65	27.4 kg/s	2.01
Air separation	Oxygen supply	0.5	0.5	21.3 kg/s	3.20
Coal gasification	Daily coal input	0.67	0.8	39.2 kg/s	5.46
Water gas shift	Material caloric Value	0.67	0.65	1377 MW	2.79
Acid gas removal	CO_2 absorption	0.67	0.65	2064.4 mol/s	2.30
Claus sulfur recovery	Sulfur output	0.65	0.7	32.5 kg/s	0.81
Gas liquid separation	Wastewater supply	0.5	0.5	0.5 kg/s	1.23
Phenol & ammonia recovery	Wastewater supply	0.5	0.5	0.25 kg/s	2.98
Back-end technology					
CTL[c]					
F-T synthesis	Syngas input	0.67	0.65	434.5 t/h	7.50
Oil hydrogenation	Oil input	0.85	0.7	138.2 t/h	5.63
SNG[d]					
Methanation	SNG output	0.65	0.65	6.95 Nm^3/s	4.94
CTO[e]					
Methanol synthesis	Syngas input	0.67	0.65	10810 mol/s	1.43
Methanol to olefins	Methanol input	0.6	1	62.5 kg/s	15.6
CTEG[f]					
H2/CO separation	H2 output	0.6	0.67	21.3 kg/s	3.21
Dimethyl oxalate synthesis	H2 input	0.65	0.65	2845.5 kmol/h	3.86
Ethylene glycol synthesis	DMO input	0.67	0.65	74.21 t/h	5.4
Ethylene glycol refinery	EG output	0.6	0.65	37.5 t/h	5.9

[a] The benchmark case data of front-end technology were obtained from references [22,29,33].
[b] In the amount of equipment investment, the US dollar was converted into CNY at an exchange rate of 7.00.
[c] The benchmark case data of CTL were obtained from references [7,12].
[d] Benchmark case data of SNG comes from reference [22].
[e] The benchmark case data of CTO were obtained from reference [19].
[f] The benchmark case data of the CTEG were obtained from reference [25].

$$C_{Fom} = C_{o\&m} + C_d + C_{ad} + C_{S\&d} \tag{9}$$

Specifically, $C_{o\&m}$ is the sum of 1) C_{wl}, the cost of labor, 2) C_{ds}, the cost of direct supervisor and clerical labor, 3) C_{lc}, the laboratory charge, 4) $C_{m\&r}$, the cost of maintenance and repairs, 5) C_{os}, the cost of operating supplies, and 6) C_{oc}, the plant overhead cost.

$$C_{o\&m} = C_{wl} + C_{ds} + C_{lc} + C_{oc} + C_{m\&r} + C_{os} \tag{10}$$

C_{wl} is calculated using Eq. (11), where C_{aver} is the average labor cost per person, N is the number of laborers, and Q is the total amount of the main product produced over the entire life period of a certain technology.

$$C_{wl} = \frac{C_{aver}}{Q} \times N \tag{11}$$

C_{ds}, C_{lc}, and C_{oc} are all human-resource-related costs that are proportional to C_{wl} by λ_{ds}, λ_{lc}, and λ_{oc}, respectively. Equipment-related costs $C_{m\&r}$ and C_{os} are proportional to *TCI* by $\lambda_{m\&r}$ and λ_{os}, respectively. These variables are expressed in Eqs. (12)-(16).

$$C_{ds} = \lambda_{ds} \times C_{wl} \tag{12}$$

$$C_{lc} = \lambda_{lc} \times C_{wl} \tag{13}$$

$$C_{oc} = \lambda_{oc} \times C_{wl} \tag{14}$$

$$C_{m\&r} = \frac{\lambda_{m\&r} \times TCI}{Q} \tag{15}$$

$$C_{os} = \frac{\lambda_{os} \times TCI}{Q} \tag{16}$$

Considering the time value of the investment, C_d in Eq. (9) is calculated using the straight-line depreciation method [34] (Eq. (17)).

$$C_d = \frac{TCI \times (1-r) \times \sum_{n=1}^{s} (1+\delta)^{n-1}}{Q} \tag{17}$$

where δ, s, and r are the discount rate, capital lifetime, and residue rate of capital, respectively.

As Eqs. (18)–(19) show, C_{ad} and $C_{S\&d}$ are proportional to PC by λ_{ad} and $\lambda_{s\&d}$, respectively.

$$C_{ad} = \lambda_{ad} \times PC \tag{18}$$

$$C_{s\&d} = \lambda_{s\&d} \times PC \tag{19}$$

2.2.3. Other indicators

To further evaluate these technologies, NPV, ROI and PP are introduced in this section, providing a more comprehensive view of their techno-economic performance. These indicators are calculated as follows.

NPV is the difference between the present value of cash inflow and cash outflow over a period and is calculated by Eq. (20) [35].

$$NPV = \sum_{t=0}^{t} \frac{CI_t - CO_t}{(1+r)^t} \tag{20}$$

where CI and CO are cash inflow and cash outflow at time t, r is the interest rate and t is the year.

The ROI is an indicator used to measure the efficiency of an investment and equals the ratio of the return on a particular investment to the amount of the investment. It can be calculated by Eq. (21) [6].

$$ROI = \frac{AR - PC \times AO}{TCI} \times 100\% \tag{21}$$

where AR is annual revenue, AO is annual output, PC is the production cost and TCI is total capital investment.

PP is the time period needed for the revenue from the investment to breakeven. It indicates the time required for an investment to make a profit. Therefore, the smaller the PP is, the better the technology performs. PP is calculated by Eq. (22) [35].

$$\sum_{t=1}^{T} CI_t - CO_O = 0 \tag{22}$$

where PP equals T, CI_t is the cash inflow at time t, and CO_O is the initial investment.

2.3. Water price scenarios

As the main production area for coal resources and coal chemical products, the northern region of China has been plagued by water shortages for a long time, which has significantly restricted economic development and the improvement of people's living standards. Water resources are becoming a limiting factor in the sustainable development of the ecological environment in this region. In the economic study of water resource management, water prices are the most basic and powerful tool that can result in the more effective use of limited water resources. Currently, the price of water (market price) is determined by the government; thus, it can hardly reflect the scarcity of water. However, existing studies on the techno-economic evaluation of MCCTs frequently use the market price to calculate the water cost of technologies while neglecting water scarcity. Moreover, they only consider the direct water cost while neglecting the indirect water cost, e.g., the cost from wastewater treatment or water infrastructure construction [19,26]. This may underestimate the potential production cost of these technologies and mislead the relevant investment activities.

To fill this literature gap and reflect how water constraints affect the techno-economic performance of MCCTs, four water price scenarios are employed in the techno-economic model:

- Scenario 1: WP1, the market price
- Scenario 2: WP2, the price considering water-related cost
- Scenario 3: WP3, the price considering water scarcity
- Scenario 4: WP4, considering both water scarcity and water-related costs

The market price of water (WP1) was obtained by averaging the industrial water prices in major coal chemical production areas, which were collected from the market survey. Detailed calculations of WP2 and WP3 are shown in Sections 2.2.1 and 2.2.2, respectively. WP4 is the combination of WP2 and WP3.

2.3.1. Water price considering the water-related cost

Water-related costs are a type of indirect cost of water and are frequently neglected in most of the literature on the techno-economic evaluation of MCCTs [9,11,33]. It consists of 1) the cost for the construction of water supply infrastructure and 2) the cost of wastewater treatment in the MCCTs.

In this study, the indirect water cost in the water price is considered by using the coefficients shown in Eq. (23):

$$P = P_{wr} \times \beta_{if} \tag{23}$$

where P_{wr} is the water price without considering the water-related cost. Specifically, P_{wr} can be either the market or shadow price of water resources. β_{wr} is a composition coefficient that reflects the ratio of the water price considering the water-related cost to P_{wr}. β_{wr} is decided by 1) β_{if}, the coefficient considering the construction cost of water supply infrastructure, and 2) $\beta_{wt}$the coefficient considering wastewater treatment cost.

2.3.2. Water price considering water scarcity

The shadow price is widely used to assess resource scarcity and the creation of environmental policy [36–38]. Using the method proposed by Liu and Chen [39], this paper calculated the shadow price of water and used this price to reflect the water scarcity in the techno-economic evaluation model. Based on China's latest input-output data [40] and water resource consumption data [30,41], the shadow prices of different industrial sectors in China were calculated. The shadow price of water resources can be obtained by solving the following linear programming model:

$$MaxZ = \sum_{n=1}^{N} a_{vn}x_n (n = 1, 2, \ldots, N) \tag{24}$$

$$a_{wn}x_n \le w_n \tag{25}$$

$$\sum_n w_n \le w \tag{26}$$

$$(I - A)X \le Y \tag{27}$$

where the objective function, Z, in Eq. (24) maximizes the total value added of all sectors, a_{vn} is the added-value factor of sector n ($n = 1, 2, \ldots, N$), and x_n is the output of the corresponding sector.

The objective function is subjected to a set of constraints. First, the water consumption of each sector should not exceed the upper limit of the corresponding sector's available water. In Eq. (25), a_{wn} and w_n are the water use coefficient and upper limit of water consumption of sector n, respectively. Moreover, the total water consumption of all sectors should not exceed the amount of water available in a certain region (w) (Eq. (26)).

Second, the objective function is subjected to the relationship between the output and final demand of the input-output model. As Eq. (27) shows, the $n \times 1$ vectors X ($X = [x_1, x_2, \ldots, x_n]^T$) and Y ($Y = [y_1, y_2, \ldots, y_n]^T$) are the output and final demand of economic sectors, respectively; the $n \times n$ matrix A is the direct demand coefficient of the economic system; and I is an identity matrix ($n \times n$).

2.4. Data

For the techno-economic model, relevant data for CTL, SNG, CTO, and CTEG were obtained from previous literature, statistical yearbooks, and the Delphi method. Because of the length of the article, only briefly introducing the data used to calculate the TCI, PC, and water prices **(shadow price of water and water price considering the water-related cost)** of the four technologies is presented here, while the detailed process description and commercial operation information are placed in the Supporting **Information (SI)**.

Data to calculate the TCI indicator included 1) the ratio factors, i.e., the proportion of each component of capital investment to the equipment investment, and 2) the benchmark case for equipment investment. The ratio factors were acquired using the Delphi method, and the results are shown in Table 2. To make the techno-economic results more comparable among the four MCCTs, this paper selected benchmark scenarios for equipment investment based on the same front-end technology. Relevant data were collected from the literature and are shown in Table 3.

Data to calculate the PC indicator included 1) technological parameters, e.g., material consumption of the production process and 2) prices of raw materials and some ratio parameters. The technological parameters were collected from existing literature and are listed in Table 4; other parameters were obtained through chemical industry yearbooks [42] and the Delphi method, as listed in Table 5.

3. Techno-economic analysis results under different water price scenarios

Based on the above methods and data, the techno-economic performances of these four types of MCCT at different scales under the four water price scenarios were evaluated. As stated earlier, to make the techno-economic results of these four types of MCCTs more comparable, this study selected an annual coal consumption of 5 million tons as the standard to ensure the approximate scale of these four major MCCTs. According to the conversion, the corresponding production capacities of CTL, SNG, CTO, and CTEG were approximately 1.0 Mt/y, 1.9 billion m^3/y, 1.2 Mt/y, and 1.4 Mt/y, respectively. All the results and discussions of this study were based on these production capacities.

3.1. Water prices under different scenarios

Data for WP1, i.e., the market price of industrial water for the major coal chemical industry area, were obtained from Ref. [43] and our calculation. WP2, i.e., the shadow price of water resources, was calculated using Eqs. (24)–(27). Relevant data were collected from the latest input-output table of China [40] and the China Water Resources Bulletin 2018 [30]. MATLAB was used to solve the above optimization model to obtain the shadow price. WP3, i.e., the water price considering the water-related cost, was calculated using Eq. (23). Relevant data were acquired from previous studies [40,43–46]. Specifically, β_{if} was between 1.24. and 3.27, β_{wt} was approximately 1.49–2.73, and β_{wr} was approximately 1.72–5.00. WP4, i.e., the price considering both water scarcity and water-related cost, was calculated by integrating WP2 and WP3 together. The results for the four water prices are shown in Table 6.

As Table 6 shows, the water price was significantly affected by

Table 4
Product and raw material consumption for the main MCCTs.

Item	Unit -product[a]			
	CTL[b]	SNG[c]	CTO[d]	CTEG[e]
Input				
Coal (t)	4.09	2.66	4.10	3.17
Water (t)	11.80	5.18	30.00	24.20
Electricity (kWh)	794.67	605.33	1672.40	878.00
Steam (GJ)	25.20	5.94	8.75	10.13
Output				
Gasoline (t)	0.25	–	–	
Diesel (t)	0.75	–	–	
SNG (Nm^3)	–	1000.00	–	
Tar (kg)	–	90.53	–	
Naphtha (kg)	–	19.14	–	
Sulfur (kg)	–	20.03	–	
Ammonia (kg)	–	9.78	–	
Phenols (kg)	–	12.07	–	
Ethylene (t)	–	–	0.46	
Propylene (t)	–	–	0.40	
$C_4^{=\alpha}$ (t)	–	–	0.14	
EG (t)	–	–	–	1

f The mass data in the reference were converted to energy using the lower heat of vaporization corresponding to the pressure.
[a] The unit of CTL, CTO, and CTEG is t, while the unit of SNG is kNm3.
[b] The input and output data for CTL were obtained from Ref. [12].
[c] The input and output data for SNG were obtained from Ref. [22].
[d] The input and output data for CTO were obtained from Ref. [18].
[e] The input and output data for CTEG were obtained from Ref. [26].

Table 5
Parameter assumptions for estimating product cost.

Parameter	Meaning	Value
P_1	Coal Price	400[a] RMB/t
P_2	Water Price	3.4[b] RMB/t
P_3	Steam Price	42 RMB/GJ
P_4	Electricity Price	0.46[c] RMB/kWh
C_{aver}	Average labor cost per person	130,000 CNY/y
N	Number of laborers	CTL[d] 400, CTO[e] 300 SNG[f] 300, CTEG[g] 500 (unit: people/y)
λ_{ds}	Ratio of direct supervisory and clerical labor toC_{wl}	20%
λ_{lc}	Ratio of laboratory charge to C_{wl}	15%
$\lambda_{m\&r}$	Ratio of maintenance and repairs to TCI	1.7%
λ_{os}	Ratio of operating supplies to TCI	0.6%
λ_{oc}	Ratio of plant overhead cost to C_{wl}	72%
λ_{ad}	Ratio of administrative cost to PC	3%
$\lambda_{s\&d}$	Ratio of distribution and selling cost	2%

[a] Coal price data were obtained from Ref. [26].
[b] Water price data were obtained from the average price of industrial water in Xinjiang, Inner Mongolia, Ningxia, Liaoning, and other major coal chemical provinces.
[c] Electricity price data were obtained from the average price of industrial electricity in Xinjiang, Inner Mongolia, Ningxia, Liaoning, and other major coal chemical provinces.
[d] The number of laborers of CTL was obtained from Ref. [15].
[e] The number of laborers of CTO was obtained from Ref. [20].
[f] The number of laborers of SNG was obtained from Ref. [22].
[g] The number of laborers in the CTEG was obtained from Ref. [26].

Table 6
Water prices under different scenarios (unit: CNY/t).

Name	Market price	Price considering water-related cost	Price considering water scarcity	Price considering both water scarcity and water-related cost
Scenario	WP1	WP2	WP3	WP4
Value	3.4	7.6	26.0	57.7

considering the water-related cost and water scarcity, as WP1, WP2, WP3, and WP4 had large differences from each other. Considering the water-related cost (indirect water cost), the water price was more than 2 times the market price of water. In comparison with considering water-related costs, considering water scarcity had a more significant effect on increasing water prices, as the shadow price of water is more than 7 times the market price of water. When considering both water scarcity and water-related costs, the price of water was more than 16 times higher than the market price of water.

3.2. TCI

As the water price primarily affects the PC of the MCCT, while having a minor effect on the TCI, the TCI results are presented separately in this part. As Fig. 1 shows, the TCI values of the CTL, SNG, CTO, and CTEG at the scale of 1.0 Mt/y, 1.9 billion m^3/y, 1.2 Mt/y, and 1.4 Mt/y are 15.5 billion CNY, 13.8 billion CNY, 28.7 billion CNY, and 15.8 billion CNY, respectively. The corresponding TCIs per unit of production capacity are 15498 CNY/t, 7275 CNY/kNm^3, 23899 CNY/t, and 1269 CNY/t.

For the TCI of MCCTs under a similar amount of coal consumption, CTO is the highest, followed by CTEG and CTL, while SNG is the lowest. The main reason is that the CTO consumes less coal per unit of product, resulting in a larger scale at the same coal consumption level, which is 1.2 Mt/y and much larger than the common commercialized production capacity of approximately 0.7 Mt/y. In addition, owing to the complexity of the technology, the capital investment per unit of production capacity of CTO was the highest. A similar observation was observed with CTEG; owing to the second-lowest coal consumption per unit of product, the production capacity of CTEG under the same coal consumption amount was relatively large and up to 1.4 Mt/y, which is much larger than the current existing operational installation scale (approximately 0.3 Mt/y). Because of the low capital investment per unit of production capacity, the TCI for CTEG was similar to that of CTL, for which the corresponding production capacity was approximately 1.0 Mt/y, which was 0.3 Mt/y smaller than the production capacity of CTEG. The lowest capital investment per unit of production capacity resulting the scale of SNG under the same coal consumption level is the largest, while the TCI is the lowest. This is why the mainstream production capacity of SNG is up to 4.0 billion m^3 per year, which is much larger than the assumed scale in this study.

3.3. PC under different water price scenarios

3.3.1. PC under the market price scenario

Using the latest raw material price and market price of water, the results of the PC and structure of PC for different MCCTs are shown in Fig. 2. The PC of CTO is the highest, which is 5918 CNY/t, followed by CTL (5185 CNY/t) and CTEG (4055 CNY/t). Because of the different product units, the product cost of SNG is the lowest (2653 CNY/kNm^3).

For the structure of the PC, the costs of raw materials make up the largest proportion, which varies from 27.7% to 40.1%, followed by the cost of public utilities ranging from 20.6% to 28.2%. The depreciation cost ranks third in all cost components, accounting for 21.1%–31.1% of PC, while the rest of the cost components account for 15.9%–20.2%.

To analyze whether these MCCTs are worthy of investment, our work compared the PCs of MCCTs with the latest market prices of oil-related products. According to our investigation on prices, the average crude oil price in 2019 was $62 per barrel [47], and the corresponding prices of liquid fuel, natural gas, olefins, and ethylene glycol were 5081 CNY/t, 2222 CNY/kNm^3, 6546 CNY/t, and 3522 CNY/t, respectively. Given the PCs of MCCTs, investing in SNG and CTEG will have a significant economic risk, investing in CTO would create a profit, and investing in CTL requires the price of their competitive products to be considered.

3.3.2. PCs under different water price scenarios

As Fig. 3 shows, considering the water constraint would increase the PC of the four MCCTs. With the water price being WP1, the results for the PC of CTL, SNG, CTO, and CTEG have already been discussed in Section 3.1. Compared with the PCs at the water price of WP1, the PCs for CTL, SNG, CTO, and CTEG would increase by 1.0% (49.6 CNY/t), 0.9% (21.8 CNY/kNm^3), 2.1% (126 CNY/t), and 2.5% (101.6 CNY/t), respectively, if the water price was WP2. Furthermore, when the water price continues to increase to WP3, the increase rate for PCs would increase to 5.1% (266.68 CNY/t), 4.2% (117.1 CNY/t), 11.5% (678 CNY/t) and 13.5% (546.9 CNY/t) for CTL, SNG, CTO and CTEG, respectively. If the water price was WP4, the PCs for CTL, SNG, CTO, and CTEG would continue to increase by 12.4% (640.7 CNY/t), 10.6% (281.3 CNY/kNm3), 27.5% (1629 CNY/t), and 32.4% (1314 CNY/t), respectively, compared with WP1. In general, under the current market price of water resources, which does not consider the water constraint of MCCTs, PC would be underestimated by 12.4% for CTL, 10.6% for SNG, 27.5% for

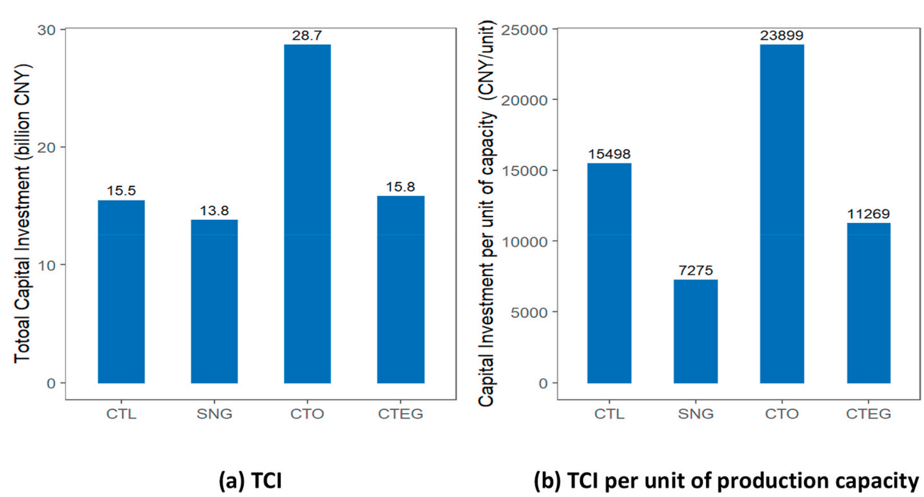

Fig. 1. TCI (a) and TCI per unit of production capacity (b) of four MCCTs.

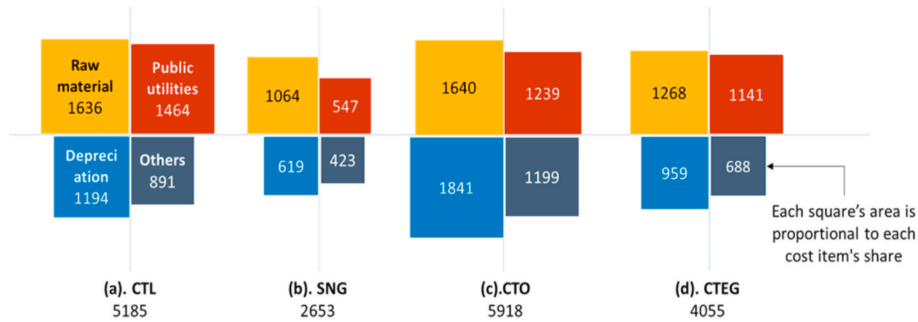

Fig. 2. PCs of different MCCTs under the market water price scenario. (The units of CTL, CTO, and CTEG are CNY/t, and the units of SNG are CNY/kNm^3).

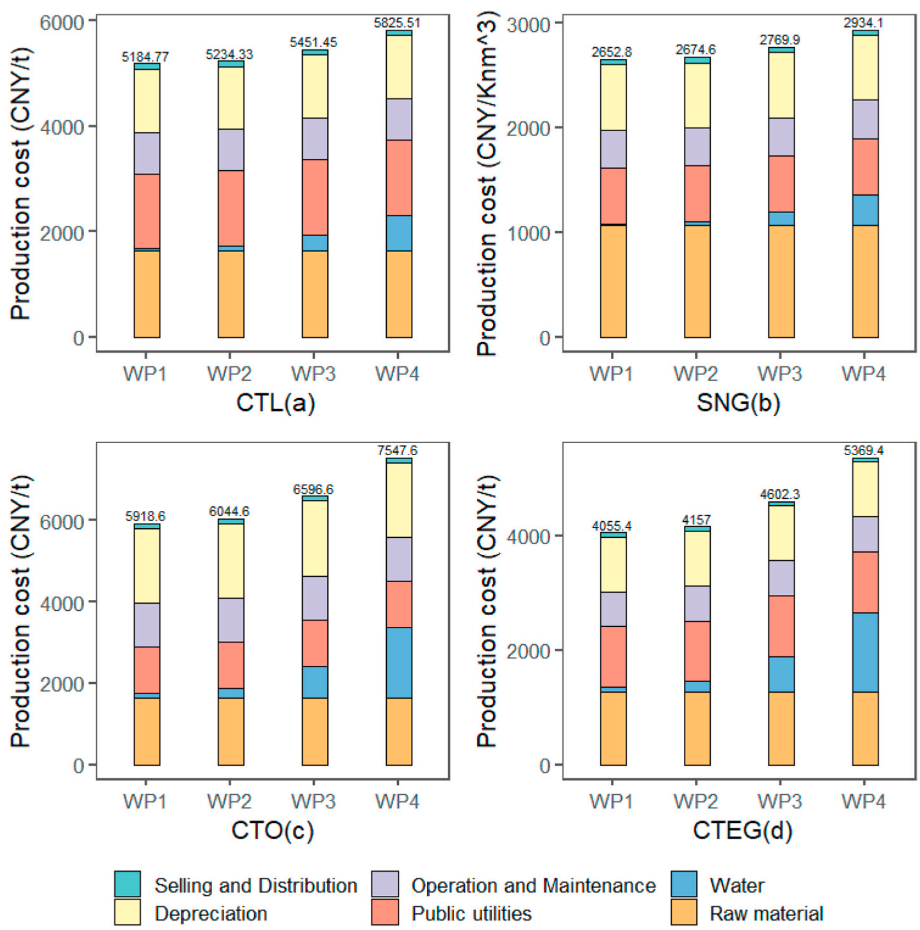

Fig. 3. Production cost of different MCCTs under four water prices: WP1, the market price; WP2, the price considering water-related cost; WP3, the price considering water scarcity; and WP4, the price considering both water scarcity and water-related cost.

CTO, and 32.4% for CTEG.

The results in Fig. 3 show that the proportion of water cost relative to PC was almost negligible for all four technologies (0.8% for CTL, 0.7% for SNG, 3.5% for CTO, and 2.0% for CTEG) when PC was considered at WP1. However, when PC was considered at WP4, the proportion of water cost relative to PC increased significantly, which was 11.7% for CTL, 10.2% for SNG, 22.9% for CTO, and 26.0% for CTEG. As a result, compared with other production costs, such as depreciation, raw material cost, and public utilities, water cost still accounts for a relatively small proportion of PC even if both water scarcity and water-related costs are considered.

3.4. Uncertainties of PCs under different water price scenarios

As discussed above, water price could be measured by the market price, the shadow price, the price considering the water-related cost, etc. These prices frequently have some uncertainties, e.g., the market price of water frequently changes with time, and the shadow price of water is calculated from the input-output table of China in 2017 due to data availability. As a result, the water cost and PC for the MCCTs have uncertainties. Therefore, this study analyzed how changes in water prices would affect the PC for the four MCCTs. These include how the PCs were affected by changes in WP1 (Fig. 4a), WP2 (Fig. 4b), WP3 (Fig. 4c), and WP4 (Fig. 4d).

The results in Fig. 4 indicate that the water price exhibited a discrepancy in the effect on the PC of all MCCTs. Among the four

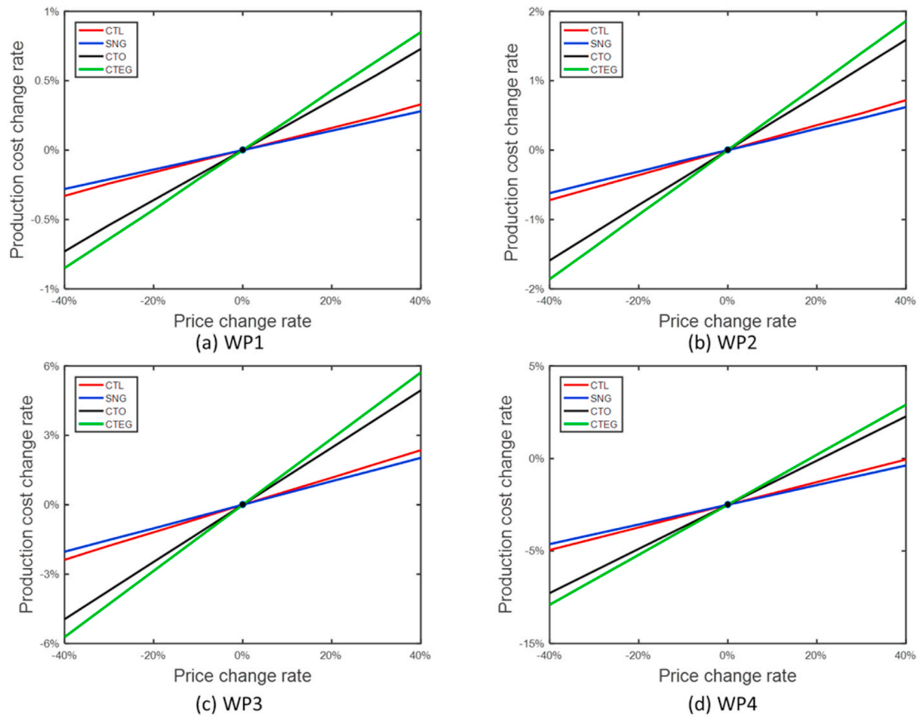

Fig. 4. Results of the sensitivity analysis of the effect of coal consumption and coal price on the PC of four MCCTs.

technologies, CTEG was the most sensitive technology, whose PC changed the most with water price, followed by CTO. Specifically, when there were ±40% changes in WP1, WP2, WP3, and WP4, the PC for CTEG changed by ±0.85%, ±1.86%, ±5.7%, and ±10.8%, respectively. The PCs for CTL and SNG had the least fluctuation with water prices, which were all lower than ±5%.

3.5. Other indicators

To better understand the techno-economic performance of MCCTs, other economic indicators were calculated. To calculate NPV, ROI and PP, the oil price is assumed to be $100 per barrel, and the market price of the products is determined by the oil price. The calculation results of NPV are shown in Table 7.

Table 7
NPV of different MCCTs when r = 6% (unit: billion CNY).

Year	CTL	SNG	CTO	CTEG
0	0	0	0	0
1	−14.6	−13.0	−27.1	−14.9
2	2.09	1.60	2.85	1.78
3	1.98	1.51	2.68	1.68
4	1.86	1.43	2.53	1.58
5	1.76	1.34	2.39	1.49
6	1.66	1.27	2.25	1.41
7	1.57	1.20	2.13	1.33
8	1.48	1.13	2.01	1.25
9	1.39	1.07	1.89	1.18
10	1.31	1.00	1.79	1.11
11	1.249	0.95	1.68	1.05
12	1.17	0.89	1.59	1.00
13	1.10	0.84	1.50	0.94
14	1.04	0.80	1.41	0.88
15	0.98	0.75	1.33	0.83
16	0.93	0.71	1.26	0.79
17	0.87	0.69	1.19	0.74
18	0.82	0.63	1.12	0.70
19	0.78	0.60	1.06	0.66
20	0.73	0.56	1.00	0.62
Cumulative NPV	10.2	5.92	6.58	6.09

The results of NPV are positive after examining the lifetimes of different MCCTs, which suggests that under a higher oil price, MCCTs have a better chance of making profits.

Based on the NPV results, the ROI and PP can also be calculated. The ROI results of CTL, SNG, CTO, and CTEG were 15.1%, 13.1%, 11.1% and 12.6%, respectively. Under an oil price of $100 per barrel, the PP for CTL is the shortest, requiring 6.59 years, followed by SNG for 7.67 years, and CTEG for 7.92 years. The PP for CTO is the longest for its largest TCI, which requires 8.98 years of operation to make the investment back.

4. Sensitive analysis of key parameters

As the parameters always have uncertainties [11,20,25,26] of the techno-economic model for MCCTs, exploring how the results of TCI or PC would change with some key parameters by conducting a sensitivity analysis is necessary.

4.1. Production capacity scale

In the techno-economic model, TCI and PC are highly dependent on the production capacity scale. Here, this work demonstrates how changes in the scale of production capacity would affect the TCI per unit of production capacity and PC for the four MCCTs. We assumed that the scales of the four technologies would change in the range of half (−50%) to twice (+100%) their reference values. Thus, the corresponding scale of CTL, SNG, CTO, and CTEG was varied from 0.5 to 2 Mt/y, 0.95 to 3.4 KNm^3/y, 0.6 2.4 Mt/y, and 0.7 to 2.8 Mt/y, respectively.

The results in Fig. 5 indicate that all four technologies had noticeable scale effects. As Fig. 5a shows, when the scales changed from −50% to +100% of the reference values, the TCIs per unit of production capacity of CTL, SNG, CTO, and CTEG changed from 15.1% to −6.1%, 25.4% to −11.1%, 16.6% to −21.6%, and 20.31% to −10.5%, respectively. For the PC, as Fig. 5b shows, with the same range of variation for the scale, the PCs of CTL, SNG, CTO, and CTEG varied from 7.4% to −3.2%, 8.0% to −5.5%, 16.3% to −12.5%, and 9.6% to −5.1%, respectively. In general, the TCIs per unit of production capacity were more sensitive to the production scale, while the CTO was more sensitive to the

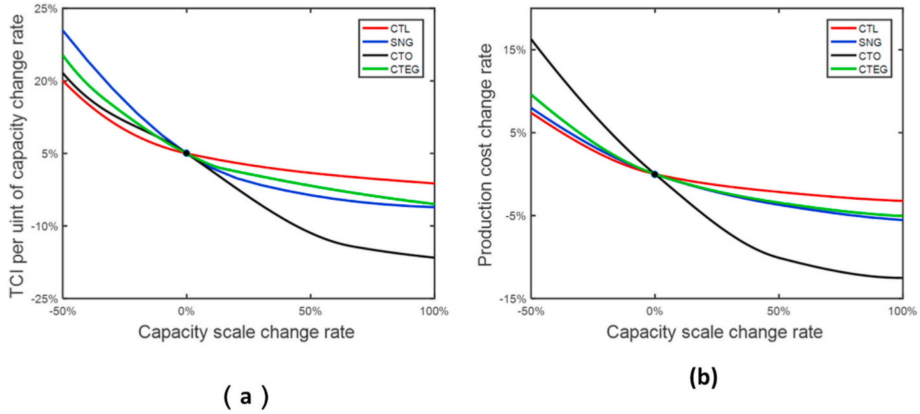

Fig. 5. Sensitivity analysis of the effect of capacity scale on TCI per unit of capacity (a) and PC (b) of MCCTs.

production scale among the four technologies compared with the PC.

4.2. Coal consumption and coal price

As a complex mixture of hydrocarbons with high impurities, the composition and properties of coal (e.g., moisture, volatilization, mechanical strength, and thermal stability) vary depending on the type of coal. Therefore, different gasifiers with very different coal consumptions have been developed for different types of coal [48], which would affect the cost of MCCTs. In addition to the consumption of coal, the price of coal changes frequently and affects the cost of these technologies [22]. Therefore, this work analyzed how the changes in coal consumption and coal price would affect the PCs for the four MCCTs.

The results in Fig. 6 indicate the following. As the coal consumption and coal price varied from 1.5 to 6.5 t/unit-product and 240 to 860 CNY/t, respectively, the PCs of CTL, SNG, CTO, and CTEG ranged from 4039 to 9269 CNY/t, 1949 to 7189 CNY/kNm^3, 4840 to 1070 CNY/t, and 3147 to 8377 CNY/t, respectively. In a more realistic scenario in which the coal consumption and coal price varied ±30% and ±50%, the PC of CTL, SNG, CTO and CTEG changed from −18.0% to 32.0% (4251.8–6859.7 CNY/t), −35.3%–38.13% (1960.6–3664.6 CNY/kNm^3), −17.1%–29.7% (5054.3–7678.3 CNY/t), and −25.5%–29.7% (3231.2–5259.2 CNY/t), respectively.

4.3. Carbon tax

Because all MCCTs are carbon intensive and under the target of carbon neutrality, it is of great importance to evaluate the carbon tax's influence on their economic performance. Therefore, in this section, a sensitivity analysis is conducted to analyze how the changes in the carbon tax would affect the PCs for the four MCCTs. At present, China has not formally implemented a carbon tax. Thus, a prediction of the carbon price of 40 CNY/t is adopted as our baseline scenario [49],and the results are shown in Fig. 7.

As shown in Fig. 7, when the baseline scenario of carbon tax is implemented, the PCs' increase rate of SNG is the largest, by 7.34% (194.8 CNY), followed by CTO, which increases 4.45% (263.2 CNY). CTEG ranks third and increased 4.13% (167.6 CNY). CTL is least

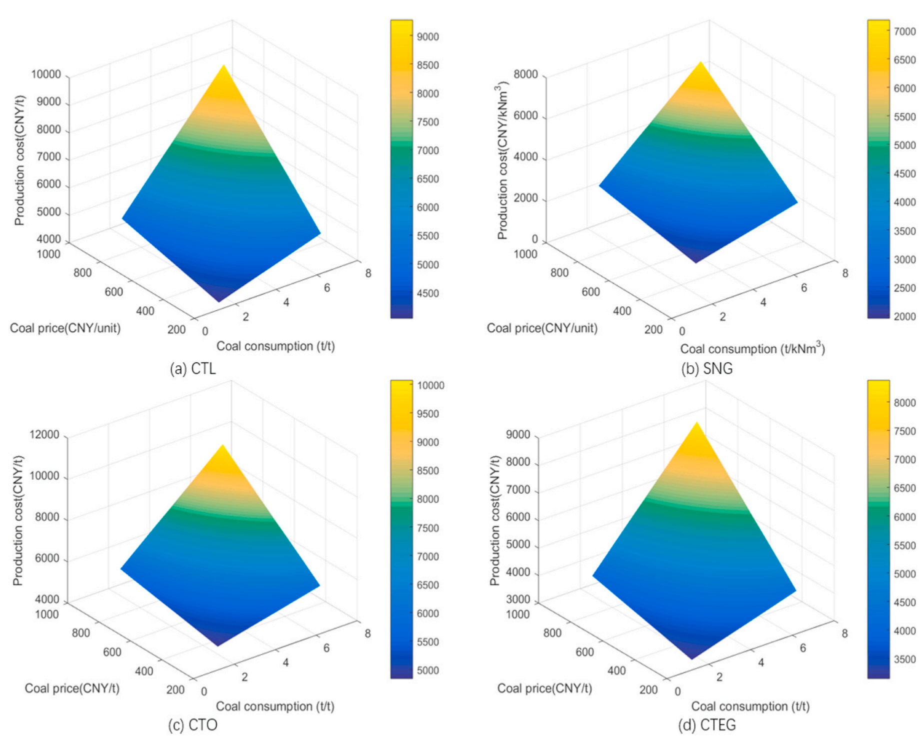

Fig. 6. Sensitivity analysis of the effect of coal consumption and coal price on the PC of MCCTs.

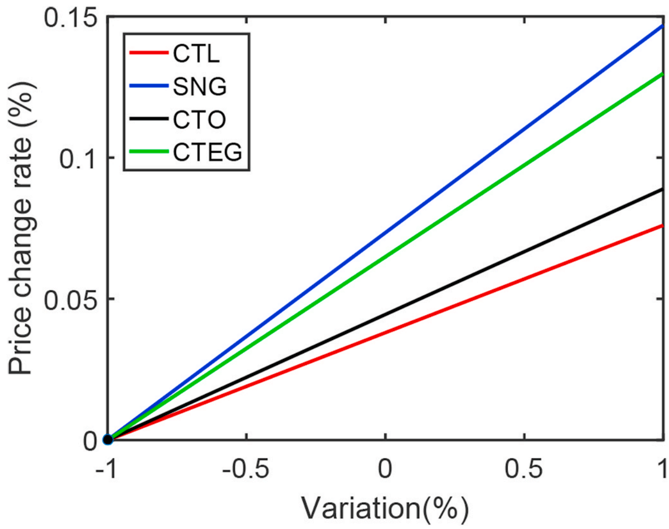

Fig. 7. Sensitivity analysis of the effect of a carbon tax on the PC of MCCTs.

influenced, only increasing by 3.8% (197.2 CNY). Although the increase in CTO is the largest, the increase rate is not. The larger base hides the increase rate. When the carbon tax is changed from −100% to 100%, which corresponds to a carbon tax from 0 to 80, the PCs for CTL, SNG, CTO and CTEG fluctuate from 0 to 7.61%, 14.69%, 8.89% and 8.27%, respectively.

5. Discussion

5.1. Profitability analysis

In this section, a profitability analysis for MCCTs is conducted; here, profitability refers to the estimation of the revenues gained from selling MCCT products in the market [35]. This profitability analysis is concluded from the comparison of current prices for oil-related products with PCs for MCCTs. The profitability of MCCTs depends primarily on the following five aspects.

1) Oil prices. Note that the prices for oil-related products will always change with oil price. The higher the oil price is, the higher the prices for oil-related products are; thus, the more profitable MCCTs will be. Since the oil price is highly uncertain and continues to fluctuate, the profitability of MCCTs always changes. For example, with the current literature's estimation, the break-even oil price of the PC of different MCCTs under the current coal price is between $50–100 barrel [12,22,26]. This indicates that under the current coal price, when the oil price is higher than $100 per barrel, MCCTs exhibit good profitability. As the oil price decreases to $50–100 barrel, the profitability of MCCTs is weakened and barely equivalent to the oil-based route. However, when the oil price is lower than $50 per barrel, it is difficult for MCCTs to profit. Therefore, future investments in MCCTs should consider long-term oil prices.
2) Coal prices. Raw material prices constitute the largest proportions of PCs for MCCTs; hence, variations in these processes have a significant effect on the PCs and profitability of MCCTs. In 2019, under an average oil price of $62 per barrel, to make a profit with CTL, SNG, CTO, or CTEG, the coal price needed to be lower than 375 CNY/t, 235 CNY/t, 545 CNY/t, and 240 CNY/t, respectively.
3) Water prices. Increasing the water price would increase the PC and thus reduce the profitability of MCCTs. If water constraints are considered in the water price, the PC would be 5286 CNY/t for CTL, 2934 CNY/kNm3 for SNG, 7548 CNY/t for CTO, and 5369 CNY/t for CTEG. None of the four MCCTs would result in a profit.
4) Production capacity scales. As mentioned earlier, the production capacity scale has a significant effect on the PCs of MCCTs; as the scale expands twice, the PCs of CTL, SNG, CTO, and CTEG decrease by 3.2%, 5.5% 12.5%, and 5.1%, respectively. This means that profits will increase (or losses will decrease). However, expanding scales would dramatically increase TCI and cause larger economic risks.
5) Conversion rates. As the prices of raw materials remain unchanged, the conversion rates of raw materials and energy efficiency become the key factors that affect PCs. The higher the raw material conversion rates and energy efficiency are, the higher the profitability of MCCT products. Moreover, to decrease production costs and improve the profitability, the future development of MCCTs should focus more on system integration and optimization, as it can reduce the cost of public utilities such as water and electricity.

Even though MCCTs may create profits, compared with oil-based routes, their payback periods are relatively longer, and their TCIs are much higher (Table 8). Considering future changes and uncertainty in oil and coal prices, the large investment in MCCTs may encounter high risks.

5.2. Policy implications

As country's strategic technological reserve for energy security, profitability and total capital investment are not the top priorities for evaluating these technologies. While investment recommendations should focus on more comprehensive aspects, such as water constraints and environmental regulations, this study compared the major techno-economic indicators, resource consumption indicators, and environmental performance indicators among the four MCCTs. These indicators include TCI, PC, coal consumption, water consumption, electricity consumption, and CO_2 emissions per unit of product. For a better comparison, indicators are normalized using the widely used min-max normalization method [26]. After normalization, all indicators ranged in [0, 1], and a lower value indicated better performance of the indicator.

As Fig. 8 shows, the four mainstream MCCTs have their advantages and disadvantages in terms of performance on different indicators. Although CTO was considered the most profitable technology of the four MCCTs, it performed the worst in almost all six indicators. This indicates that CTO is the technology most affected by the water constraint, as it requires the highest water consumption. In addition to focusing on the large capital investment and water constraints, future investments in

Table 8
Techno-economic comparison of MCCTs with oil-based technologies.

Products	PC[a]			TCI[b]	
	MCCTs (Coal price: 400 CNY/t)	Oil-based routes (Oil price: $62 barrel)	Breakeven coal prices (Unit: CNY/t)	MCCTs	Oil-based technology
Liquid fuel	5185	5081	375	15498	2578[c]
Natural gas	2653	2222	235	7275	2310[d]
Olefins	5918	6546	545	23899	8400[e]
Ethylene glycol	4055	3522	240	11269	6536[f]

[a] The unit of PC for CTL, CTO, and CTEG is CNY/t, while the unit of SNG is CNY/kNm^3.
[b] The unit of TCI for CTL, CTO, and CTEG is CNY/t/y, while the unit of SNG is CNY/kNm^3/y.
[c] The TCI data of liquid fuel for oil-based options come from Ref. [12].
[d] Natural gas is a type of primary resource, the domestic extracting cost is used instead of TCI, and the data were obtained from Ref. [22].
[e] The TCI data of olefins for oil-based options come from Ref. [9].
[f] The TCI data of ethylene glycol for oil-based options come from Ref. [26].

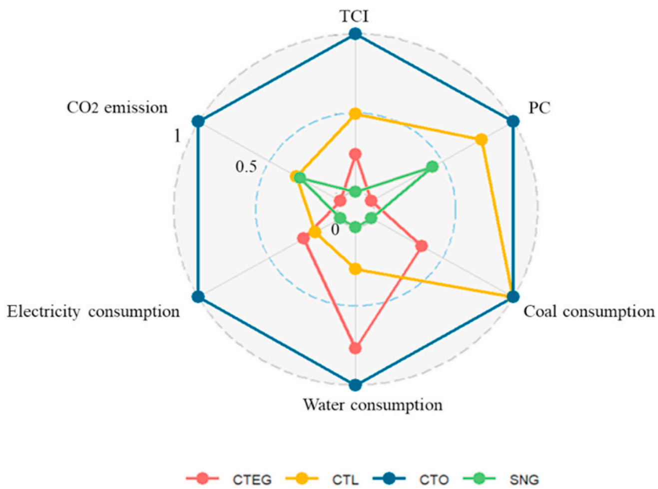

Fig. 8. Comparison of different indicators for CTO, CTL, CTEG, and SNG. [a] The CO2 emission data were obtained from Ref. [50].

CTOs should focus more on the prices of materials and environmental policies and the need for more time to pay back the investment. On the one hand, because of the highest consumption of coal and electricity, the profitability of CTO would be most significantly affected by the changes in the prices of coal and electricity. On the other hand, because of the highest CO_2 emissions, the profitability of CTO would most likely be affected when stricter environmental policy (e.g., higher carbon tax) is implemented.

In contrast to CTO, SNG performed the best in almost all six indicators, except for CO_2 emissions and PC. However, investment in SNG requires consideration of its pollution and the prices of competitive technical routes. In addition to a large economic risk, CTL performed the worst on coal consumption and the second-worst on TCI, PC, and CO_2 emissions. However, the consumption of water and electricity for CTL was relatively good. As a result, CTL is less affected by water constraints and is more likely to be affected by coal prices and environmental policies. CTEG had the best performance in terms of CO_2 emissions and the second-best performance on TCI, PC, and coal consumption while consuming large amounts of water and electricity.

In summary, considering only current profitability, CTO is the best option for investment. However, investors should be cautious, as CTO has the highest TCI, and its profitability would be mostly affected by water constraints, environmental policies, and material prices. Considering only the cost of investment, CTEG and SNG are good options, while CTL and CTO both require large amounts of capital investment. When water constraints are given top priority, SNG is the best choice for investment, followed by CTL. When environmental protection, particularly CO_2 emissions, is the primary consideration, CTEG is the most preferred option, followed by CTL and SNG.

6. Conclusion

As an alternative to petrochemical technology, MCCT has been recognized as a strategic reserve technology for national energy security and will contribute significantly to the energy supply system in China. However, its profitability and environmental effects (particularly water constraints) have long been disputed. In this study, coupled with models that consider water scarcity and indirect water cost, a classical techno-economic evaluation model was adopted to evaluate the performance of different MCCTs under water constraints. In addition, the sensitivity of the results to some key parameters is discussed in this paper. Investment recommendations are also provided considering profitability, cost of capital investment, material consumption, water constraint, and CO_2 emissions. The main conclusions are as follows:

- With the current raw material price, the TCIs per unit production capacity of CTL, SNG, CTO and CTEG are 15498 CNY/t, 7275 CNY/kNm^3, 23899 CNY/t, and 1269 CNY/t, respectively, while their production costs are 5185 CNY/t, 2653 CNY/kNm^3, 5918 CNY/t and 4055 CNY/t, respectively. Compared with the current prices of oil-related products, investing in SNG and CTEG carries a significant economic risk, investing in CTL can barely make a profit, while investing in CTO could make a profit. Investors should be cautious, as profitability is highly dependent on the current prices of oil and coal.
- Under the current market price of water resources, which does not consider the water constraint of MCCTs, the production cost would be underestimated by 1.0–12.4% for CTL, 0.8–10.6% for SNG, 2.1–27.5% for CTO, and 2.5–32.4% for CTEG.
- When water constraints are given top priority, SNG is the best option for investment since its cost fluctuates the least (0.82%–10.6%) after the water scarcity price is considered. CTL ranks second (0.96%–12.4%). Environmental protection, particularly CO_2 emissions, is the primary consideration, and CTEG is the most preferred, followed by CTL and SNG.

Credit author statement

Jinyang Zhao: Resources, Writing – original draft, Methodology, Investigation, Visualization. Li Zhou: Investigation, Data curation. Wenji Zhou: Methodology, Data curation. Hongtao Ren: Methodology, Validation. Yadong Yu: Conceptualization, Writing – review & editing, Funding acquisition. Fucheng Wang: Investigation, Data curation. Tieju Ma: Conceptualization, Writing – review & editing, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at https://doi.org/10.1016/j.esr.2021.100754.

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