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Intensive carbon dioxide emission of coal chemical industry in China

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HIGHLIGHTS

- Local CO_2 emission factors of China’s coal chemical products are published.
- The total CO_2 emission from China's coal chemical industry was 607 Mt in 2015.
- The spatial disparity of CO_2 emission from China's coal chemical industry is great.
- CO_2 emission from modern coal chemical industry is predicted to be 417 Mt in 2020.
- Carbon capture, utilization, and storage has great potential to reduce its emission.

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ABSTRACT

As the largest producer of coal chemical products in the world, China faces tremendous pressure to reduce its carbon emission. An accurate quantification of the carbon dioxide (CO_2) emission of coal chemical industry in China is therefore necessary. However, due to the variety of coal chemical products and limitations of CO_2 emission factors, the total CO_2 emission of coal chemical industry has yet to be determined. In this study, local CO_2 emission factors of coal chemical products in China are published based on first hand data from twenty-three coal chemical enterprises and the total CO_2 emission of China's coal chemical industry is extrapolated. The provincial-level spatial distribution of the CO_2 emission of coal chemical industry is presented to assist the government in identifying key emission reduction areas. Additionally, scenario analysis of CO_2 emission for China’s modern coal chemical industry in 2020 is conducted to determine whether the development of the modern coal chemical industry will have a significant impact on future CO_2 emission, as well as the effect of carbon capture, utilization and storage technologies on the reduction in carbon emission. The estimate shows that the total CO_2 emission of the coal chemical industry in 2015 was 607 million tonnes (Mt), accounting for approximately 5.71% of China’s total CO_2 emission. The figure is higher than the total annual CO_2 emission of a country such as Canada (555 Mt) or Brazil (486 Mt). Quantifying the emission of the coal chemical industry is therefore critical to understand the global carbon budget. The spatial distribution shows that Shandong, Inner Mongolia and Shanxi release one-third of the coal chemical industry’s total CO_2 emission. Considering the development of the modern coal chemical industry, its CO_2 emission is predicted to be as high as 416.52 million tonnes in 2020. However, the CO_2 emission could be reduced by 317.98 million tonnes when carbon capture, utilization and storage are applied to process and energy systems simultaneously. This paper quantifies the CO_2 emission of the coal chemical industry in China for the first time, identifies key chemical products and the provinces in which they are produced, explores the carbon reduction potential by scenario analysis, and provides specific data to support the assessment of effective CO_2 reduction policy.

1. Introduction

With the continuous growth of China’s economy and better living conditions for citizens, there is a significant rigid demand for clean oil, natural gas and other coal chemical products (CCPs). Unlike many other countries that produce these chemicals by transforming oil or natural

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gas, China relies primarily on coal as the feedstock due to its abundant coal resource and relatively scarce oil and natural gas reserves [1]. The imports of petroleum and natural gas accounted for 65.4% and 33.5% of China's total consumption in 2016, respectively [2]. Furthermore, considering the volatility of international crude oil prices and scarcity of domestic crude oil and natural gas, the coal chemical industry (CCI) is of far-reaching significance for the national energy strategy, which can convert coal to oil or synthetic natural gas (SNG). CCI has become an important pillar industry, also drives the development of other Chinese industries. According to the maturity of its development, CCI is classified as traditional CCI or modern CCI in China. Nowadays, China is the largest producer of traditional CCPs in the world. The production of methanol, ammonia and coke account for approximately 28%, 32%, 58% of global production, respectively [3]. During the *Twelfth Five-Year* period, the industrial scale of modern CCI expanded rapidly and, according to government plans, still has broad prospects for development in the future [4].

However, as one of the most important sectors for coal use, CCI is also a leading contributor to carbon dioxide (CO_2) emission [5]. The processes of coal gasification and coal liquefaction, which are the main routes from coal to chemicals, are also major sources of CO_2 in China. When coal is used as raw material to produce chemicals, the CO_2 emission is more intensive due to the higher carbon/hydrogen ratio as compared to petroleum or natural gas. The emission factor of coal-based ammonia in China is 4.6 tonnes CO_2/tonnes NH_3, which is much higher than natural gas-based (2.1 tonnes CO_2/tonnes NH_3) and oil-based (3.3 tonnes CO_2/tonnes NH_3) [6]. The same result is also found in Australia's ammonia plants [7]. Considering the haze pollution in Chinese cities during cold periods, which is chiefly attributable to coal-based municipal heating, the use of coal-based synthetic natural gas (SNG) to replace coal for municipal heating is conductive to mitigating haze pollution in metropolitan areas. However, Li et al. found that it comes at the expense of consuming 90% more coal and emitting 65% more GHG (greenhouse gas) than the coal heating route from the life cycle perspective [8]. Similarly, the SNG electricity generation produces more GHG than traditional coal-fired electricity generation, up to 2.6–3.3 times the levels associated with the conventional natural gas pathway [9].

In 2016, China signed the Paris Agreement and promised to reduce its emission of CO_2 per GDP (gross domestic product) by 40% to 45% from 2005 levels by 2020—a commitment that requires an ambitious mitigation plan. To set up a reasonable carbon reduction plan, China must build a complete CO_2 emission inventory of all sectors. Nowadays, there are many estimations of China's CO_2 emission from different perspectives. Zhao et al. estimated China's CO_2 emission from the bottom up based on a detailed categorization of economic sectors and provincial economic and energy data [10]. Wang et al. estimated China's CO_2 emission from the both production and consumption perspectives and revealed that nearly 25% national emission were caused by net exports [11]. Beyond that, some studies focused on key CO_2 emission industries, including fossil fuel combustion [12], industrial materials production [13], cement industry [14], lime industry [15], and the iron and steel industry [16]. For example, Cai et al. evaluated the overall CO_2 emission of China's cement industry based on detailed information on China's 1574 cement enterprises [17]. Based on aforementioned estimations, a number of in-depth studies on carbon reduction potential were conducted. Considering the high CO_2 emission of electricity consumption in China's chemical industry, Yue et al. modeled the benefit of electricity savings for CO_2 emission reduction from the industry on power grid level [18]. An et al. analyzed the effectiveness of four different strategies on the potential of CO_2 emission reduction to provide a more flexible technology development path for the iron and steel industry [19]. These studies provide specific support for CO_2 emission reduction policies in different industries. However, few considered CCI as an independent sector, thus greatly reducing the accuracy of the CO_2 emission inventory.

It is more difficult to estimate the CO_2 emission of CCI as compared with other industries for two reasons. First, there are different types of CCI products and the statistical data of annual outputs are not accurately known in China. This is especially the case for modern CCI, which is only developed recently: official statistics are not yet sound. Second, localized emission factors are deficient for CCPs. The emission factors (EFs) recommended by the Intergovernmental Panel on Climate Change (IPCC) [20] have been widely applied to calculate CO_2 emission by various industries. However, the CO_2 emission factors of most CCPs are not included in the IPCC EFs since the EFs of these chemicals are based on crude oil or natural gas as a raw material. In order to fill the data gap, the quantification of the CO_2 emission factor was examined for a single CCP, such as methanol [21], coke [22] and SNG [23]. However, most studies are based on secondary data, which mean lower credibility [24]. Others are based on Aspen Plus simulation [25], which may be different from actual production. To our knowledge, no study has been published on the CO_2 emission factors of coal-to-ethylene glycol and coal-to-oil (direct liquefaction). Thus, this study will fill the gap in the quantification of the CO_2 emission from coal chemical industry.

This research aims to (i) calculate the local CO_2 emission factors of CCPs in China based on first-hand data from twenty-three coal chemical enterprises, (ii) estimate the total CO_2 emission of China's CCI, (iii) determine the spatial disparity of CO_2 emission from CCI among provinces, and (iv) evaluate the impact of carbon capture, utilization, and storage (CCUS) technologies on the carbon emission reduction of modern CCI in China in 2020. Furthermore, we calculate the CO_2 emission from Chinese chemical products by considering other alternative feedstock such as petroleum and natural gas, and compare it with that of CCI. The uncertainty is analyzed with Monte Carlo simulation, and the results of EFs are further compared with existing studies.

2. Methodology and data sources

2.1. System boundaries

Eleven main coal chemical production processes and products are considered, as shown in Fig. 1. Traditional CCI includes coal-to-coke, coal-to-ammonia, coke-oven gas-to-methanol, coal-to-urea and coal-to-methanol, while modern CCI includes coal-to-ethylene glycol, coal-to-oil, methanol-to-olefin, coal-to-olefin and coal-to-natural gas.

The life cycle assessment studies of certain coal chemical products including olefins [21], SNG [26] and methanol [27] show that the upstream materials production process is not the major contributor to the total CO_2 emission. For example, Qin's estimation shows that the upstream process of coal supply only contributes 4.3% of life cycle CO_2 emission of the coal-to-methanol chain [25]. We intend to emphasize coal use and its resulting CO_2 emission for the industry. Therefore, the system boundaries of this study include the production processes of CCPs, upstream electricity and steam production, irrespective of the upstream production of raw material and fuel. The system boundary we defined is also consistent with the *Guidelines for Accounting and Reporting Greenhouse Gas Emission for Chinese Chemical Production Enterprises*, which are issued by the Chinese government [28].

The CO_2 released by coal chemical production may be categorized into two sources. One occurs in the conversion process from feedstock to final product, defined as process system emission. The other is caused by energy consumption, defined as energy system emission. All process system emission is identified as direct emission, while energy system emission include direct emission from on-site fuel combustion and indirect emission from upstream energy production including electricity and steam.

2.2. Calculation method

Based on the data for coal chemical enterprises, we calculate the emission factors of CCPs, and then estimate the total CO_2 emission of

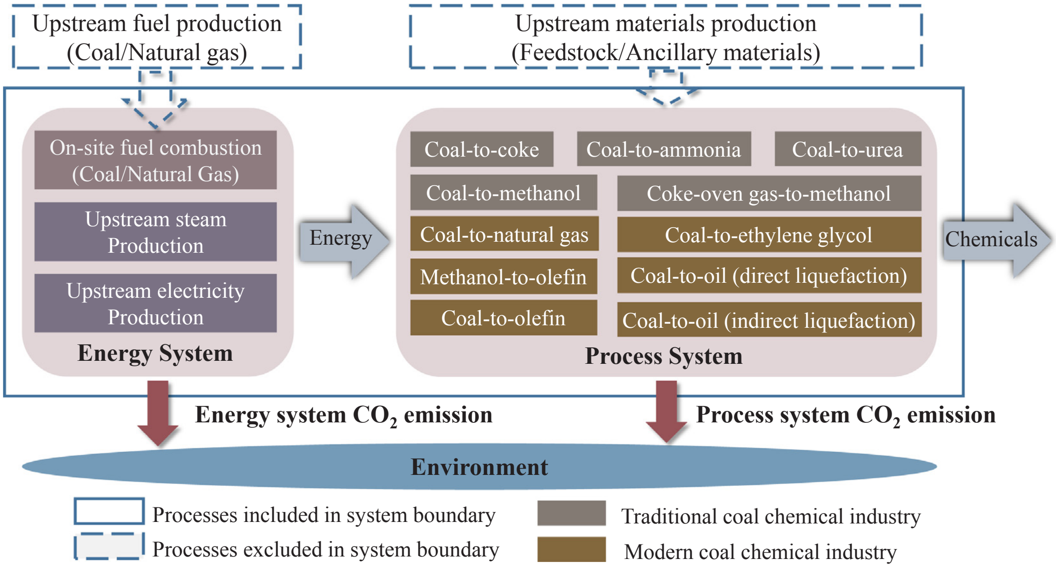

Fig. 1. System boundary of the CO_2 emission calculation.

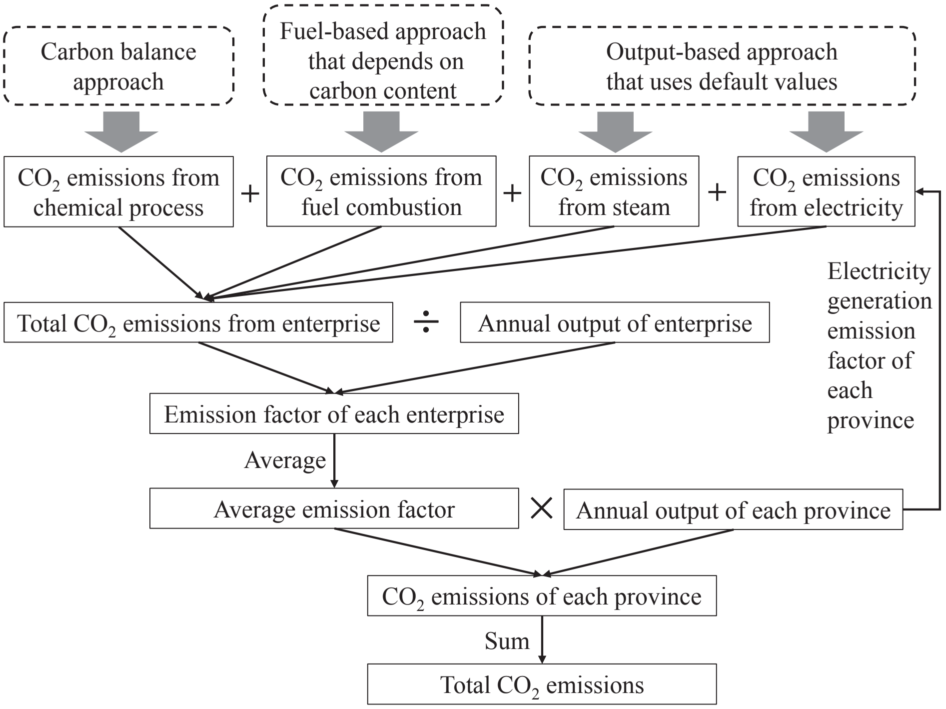

Fig. 2. Schematic diagram of data process.

CCI by integrating the EFs and the annual outputs of each province, as shown in Fig. 2.

2.2.1. Calculation of the CO_2 emission factors of coal chemical products

We consider four sources of CO_2 emission of coal chemical enterprises, including chemical processes, fuels combustion, electricity consumption and steam consumption. We first calculate the emission factors of each enterprise according to Eqs. (1) and (2).

$$E_{kij-total} = E_{ki-process} + E_{ki-burning} + E_{kij-electricity} + E_{ki-\mathrm{steam}} \tag{1}$$

$$EF_{kij} = \frac{E_{kij-total}}{Q_{ki}} \tag{2}$$

where $E_{kij-total}$ is the total CO_2 emission of enterprise k, which produced chemical i with a specific technology in province j; $E_{ki-process}$ is the CO_2 emission of the chemical processes; $E_{ki-burning}$ is the CO_2 emission of fuels combustion; $E_{kij-electricity}$ is the CO_2 emission of the net purchase of electricity; $E_{ki-\mathrm{steam}}$ is the CO_2 emission of the net purchase of steam; EF_{kij} is the CO_2 emission factor of enterprise k and Q_{ki} is the annual output of enterprise k.

Then, the average emission factor of several coal chemical enterprises is taken as the final EF of CCP, as shown in Eq. (3).

$$EF_{ij} = \frac{\sum_{k=1}^{n} EF_{kij}}{n} \tag{3}$$

where EF_{ij} is the CO_2 emission factor of chemical i with a specific technology in province j; EF_{kij} is the CO_2 emission factor of enterprise k and n is the number of enterprises that produce chemical i with a specific technology.

We also calculate the average emission factor of each coal chemical process and product in China based on the above calculation results, as shown in Eq. (4).

$$EF_{i-average} = \frac{\sum_{j=1}^{31} (EF_{ij} \times Pro_{ij})}{\sum_{j=1}^{31} Pro_{ij}} \tag{4}$$

where $EF_{i-average}$ is the average CO_2 emission factor of chemical i with a specific technology, Pro_{ij} and EF_{ij} are the output and CO_2 emission factor of chemical i with a specific technology in province j in 2015, respectively.

(1) Process system emission

The calculation of the CO_2 emission of the process system is based on the mass balance of carbon element, as shown in Eq. (5). Considering the unavailability of data, the carbon element in wastewater is ignored and we assume all carbon element in exhaust gas is emitted as CO_2. The assumption has little impact on the result because the amount of carbon emitted by wastewater and the other carbon-containing substances in the exhaust gas is rare based on our study of coal chemical enterprises. Furthermore, part of the other carbon-containing substances in the exhaust gas, such as CO and CH_4, will be burned through the high-pressure torch in the actual process, converted into CO_2 and emitted into the atmosphere. It should be noted that methanol is the raw material of methanol-to-olefin, which contributes little CO_2 emission in the chemical processes, so the CO_2 emission of its chemical processes is not considered.

$$E_{ki-process} = \left\{\sum\nolimits_r (AD_r \times CC_r) - \left[\sum\nolimits_p (AD_p \times CC_p) + \sum\nolimits_w (AD_w \times CC_w)\right]\right\} \times \frac{44}{12} \tag{5}$$

where r is the type of raw material; AD_r is the input amount of raw material r; CC_r is the carbon content of raw material r; p is the type of product; AD_p is the output of product p; CC_p is the carbon content of product p; w is the type of waste; AD_w is the output of waste w; CC_w is the carbon content of waste w and $\frac{44}{12}$ is the ratio of the relative molecular mass of CO_2 to the relative atomic mass of a carbon atom.

(2) Energy system emission: emission of fuel combustion

The CO_2 emission of fuel combustion is calculated in Eq. (6). When the carbon content data of fuel are not available for the studied enterprises, they are estimated based on the net calorific value of the fuel, as shown in Eq. (7). The oxidation rate [28] data and carbon content factor per net calorific value [20] are the default values from the literature.

$$E_{ki-burning} = \sum\nolimits_f (AD_f \times CC_f \times OR_f \times \frac{44}{12}) \tag{6}$$

$$CC_f = NCV_f \times CF_f \tag{7}$$

where f is the type of fuel; AD_f is the input of fuel f; CC_f is the carbon content of fuel f; OR_f is the oxidation rate of fuel f; NCV_f is the net calorific value of the fuel f and CF_f is the carbon content factor per net calorific value of fuel f.

(3) Energy system emission: emission of electricity and steam consumption

Because of the difference in the electricity grid structure, we use provincial electricity CO_2 emission factors [29] to replace the emission factor of the regional electricity grid where the enterprise is located. Then, we obtain the revised emission factor of each province. The CO_2 emission of the net purchase of electricity and steam is calculated in Eqs. (8) and (9), respectively.

$$E_{kij-electricity} = AD_{electricity} \times EF_{j-electricity} \tag{8}$$

$$E_{ki-\mathrm{steam}} = AD_{\mathrm{steam}} \times EF_{\mathrm{steam}} \tag{9}$$

where $AD_{electricity}$ is the net purchase of electricity; $EF_{j-electricity}$ is the CO_2 emission factor of electricity generation in province j; AD_{steam} is the net purchase of steam and EF_{steam} is the CO_2 emission factor of steam.

2.2.2. Calculation of total CO_2 emission of CCI by product

We estimate the total CO_2 emission of CCI in China by calculating the CO_2 emission of eleven key coal chemical processes and products in each province respectively, as shown in Eq. (10). The CO_2 emission factors are calculated using data from the studied coal chemical enterprises.

$$T_{CO_2} = \sum_{j=1}^{31} \sum_{i=1}^{11} (Pro_{ij} \times EF_{ij}) \tag{10}$$

where T_{CO_2} is total CO_2 emission of CCI; Pro_{ij} and EF_{ij} are the output and CO_2 emission factor of chemical i with a specific technology in province j in 2015, respectively.

Based on the annual output data of coal chemical products, the total CO_2 emission of each product is calculated by aggregating the provincial emission, as shown in Eq. (11).

$$I_{CO_2-i} = \sum_{j=1}^{31} (Pro_{ij} \times EF_{ij}) \tag{11}$$

where I_{CO_2-i} is the total CO_2 emission of product i with a specific technology.

2.2.3. Calculation of CO_2 emission of CCI in each province

In order to analyze the distribution characteristics of CO_2 emission of CCI, we calculate the total CO_2 emission of each province by aggregating the emission of all products, as shown in Eq. (12).

$$J_{CO_2-j} = \sum_{i=1}^{11} (Pro_{ij} \times EF_{ij}) \tag{12}$$

where J_{CO_2-j} is the total CO_2 emission of province j.

2.3. Data sources

2.3.1. Data sources used to estimate emission factors

(1) Data from coal chemical enterprises

We collect firsthand data on twenty-three coal chemical enterprises by conducting a field study and analyzing environmental impact assessment and environmental monitoring reports. In the investigation of coal chemical enterprises, we use a combination of site surveys, interviews with engineers and questionnaires. Then, we create the standardized inventory for each enterprise (see supplementary material for detailed data), which includes all the processes and products within the study boundaries, as shown in Fig. 1.

(2) Data from literatures

As for the missing data in the survey, such as the carbon content of tar, they are supplemented by data found in the literature [30]. Detailed parameters for each enterprise are in Table S2. China's regional electricity grid is divided into northeast China, north China, east China, central China, northwest China and south China, as shown in Table S1. The CO_2 emission factor of electricity generation for each regional electricity grid is taken from government documents [29].

Table 1
CO_2 emission factors of different coal chemical products in China (Unit: t CO_2/t product; 95% Confidence Interval).

	Coal chemical product	Process system	Energy system			Total
			Electricity-related	Fossil fuel-related	Steam-related	
Traditional CCI	Coal-to-coke	0.12	0.035	0.033	0.027	0.22 (0.20–0.23)
	Coal-to-ammonia	3.14	0.52	0.78	0	4.44 (4.23–4.66)
	Coal-to-urea	1.75	0.18	2.29	0	4.23 (3.82–4.62)
	Coke-oven gas-to-methanol	0.32	0.14	0	0.02	0.48 (0.38–0.58)
	Coal-to-methanol	2.55	0.17	1.55	0	4.27 (4.00–4.52)
Modern CCI	Coal-to-olefin	6.58	1.64	2.37	0	10.6 (10.1–11.1)
	Methanol-to-olefin	0	0.23	2.60	0	2.83 (2.62–3.05)
	Coal-to-ethylene glycol	4.19	0.38	5.91	0	10.5 (9.5–11.5)
	Coal-to-natural gas	4.87	0.15	1.50	0.059	6.58 (6.05–7.12)
	Coal-to-oil (direct liquefaction)	2.93	0	1.09	0	4.03 (3.02–5.02)
	Coal-to-oil (indirect liquefaction)	4.93	0.67	2.07	0	7.67 (6.83–8.54)

2.3.2. Data sources for the provincial annual outputs of coal chemical products

There are two main sources to acquire the annual output data of coal chemicals in each province. Since traditional CCI is fully developed, the annual output data of traditional coal chemical chemicals are based on official statistics such as the national statistical database [31] and industry association statistics [32]. Modern CCI has only been developed for a few years. On one hand, the official statistics are not yet sound. On the other hand, the number of modern coal chemical enterprises is relatively low. As a result, we could only collect the annual output data of coal chemical enterprises on an individual basis through web data mining. For example, since coal chemical enterprises are mostly subsidiaries of listed companies, we are able to obtain production information in their annual reports. We could also get the annual output data of modern coal chemical from local government reports, apply to local governments for information and so on. Finally, the official data on national total production [4] are used to calibrate the summary data of all provinces. The detailed data of provincial annual output are shown in the supplementary material.

2.3.3. Explanation of data sources

Because of the limited availability of the data, we only collect firsthand data from twenty-three coal chemical enterprises. These coal chemical enterprises make up five of China's top ten coal chemical companies. For example, the coal-to-oil enterprises from which we acquired produced 90% of China's coal-based oil in 2015 [4]. The process data also cover a range of representative technologies. For example, atmospheric fixed bed intermittent gasifier technology is the main gas technology used to produce ammonia and methanol [32]. The Claus process method is the most widely used sulfur recovery technology in CCI [33]. Direct liquefaction and indirect liquefaction technologies are used to transform coal to oil in China [34]. In addition, we compare our CO_2 emission factors with existing studies in the results to verify the reliability of our survey data.

2.4. Uncertainty analysis

The uncertainty of the estimations for the CO_2 emission factors of coal chemical products and total CO_2 emission of CCI in China in 2015 is quantitatively evaluated with Monte Carlo simulation. Since the annual output data of coal chemical products are mainly taken from official statistics and detailed summary of each coal chemical plants, thus we assume that these data had no uncertainty in emission estimation. The inventory of each enterprise, including input and output data, is based on the actual process data. Therefore, it is assumed that there is no uncertainty in this part, either. Nevertheless, there is uncertainty with regard to the parameters used in the calculations. For example, the chemicals involved in the chemical process are basically mixtures. If only a single carbon content is used, it can bring great uncertainty to the results. It is thus necessary to quantify the uncertainty of these parameters.

As most of the parameters have only one value due to the scarcity of information, parameters are provided with uniform distribution by taking data quality into account as the possibility of appearance. Coefficients of variation (CVs) are set according to the qualitative assessment of their data qualities and subject judgement. Probability distributions of these parameters for all enterprises are shown in Table S2. A total of 10,000 Monte Carlo simulations are performed to quantitatively test the propagation of input uncertainty into the final results at the 95% confidence interval.

Theoretically, it will be perfect to collect the production data of all coal chemical enterprises in China, by which CO_2 emission factor could be calculated with weighted arithmetic mean on the basis of their output data of chemical products. However, due to limited availability of data, the arithmetic mean of several coal chemical enterprises is taken as the final emission factor of coal chemical product, which is also a source of uncertainties in this study. In order to demonstrate the uncertainty generated by the limitation, the emission factors of different enterprises are compared in Table 2.

3. Results

3.1. CO_2 emission factors of coal chemical products in China

The average emission factors of coal chemical products in China are shown in Table 1 (see Table 2 for the detailed CO_2 emission factors of enterprises). The results infer that a majority of modern coal chemical products have higher CO_2 emission factors as compared to traditional coal chemical products. More specifically, when using coal as a raw material to produce olefin and ethylene glycol, the CO_2 emission factors are as high as 10.6 and 10.5 t CO_2/t product, respectively. Coal-to-olefin has the highest CO_2 emission factor from the process system, while coal-to-ethylene glycol has the highest CO_2 emission factor from the energy system.

Upon most occasions, the CO_2 emission factors of the process system are higher than those of the energy system, except for coal-to-urea, methanol-to-olefin, and coal-to-ethylene glycol. For most coal chemical products, including urea, methanol, olefin, ethylene glycol, SNG and oil, fossil fuel combustion is the main contributor to the CO_2 emission of energy system because the cost of electricity from the grid is much higher than coal-based captive power plants for these large-scale enterprises. At the same time, coal-based captive power plants can provide steam for chemical processes. Therefore, finding a way to decrease the number of coal-based captive power plants is the key to mitigating CO_2 emission of energy system at the policy level. Compared to coal-to-ammonia, coal-based urea transforms coal to ammonia firstly. Then the purified CO_2 from the upstream process reacts with it to produce urea. Coal-based urea therefore not only consumes CO_2 from the process

Table 2
CO_2 emission factors of coal chemical enterprises.

Product and process	Data sources	Emission factor (t CO_2/t product)
Coal-to-methanol	Enterprise A	4.368
	Enterprise B	4.144
Coal-to-oil (indirect liquefaction)	Enterprise C	7.255
	Enterprise D	7.775
Coal-to-oil (direct liquefaction)	Enterprise E	4.025
Coal-to-coke	Enterprise F	0.190
	Enterprise G	0.234
Coal-to-natural gas	Enterprise H	5.838
	Enterprise I	7.382
	Enterprise J	6.323
	Enterprise K	7.101
Coke-oven gas-to-methanol	Enterprise L	0.501
	Enterprise M	0.447
Coal-to-urea	Enterprise N	4.564
	Enterprise O	3.885
Coal-to-ammonia	Enterprise P	4.050
	Enterprise Q	4.834
Coal-to-ethylene glycol	Enterprise R	6.012
	Enterprise S	5.810
Coal-to-olefin	Enterprise T	11.790
	Enterprise U	8.865
	Enterprise V	10.835
Methanol-to-olefin	Enterprise W	2.808

system but also requires more energy. This is why the CO_2 emission of the process system is lower than that of the energy system. Coal-to-coke, coke-oven gas-to-methanol and methanol-to-olefin have much lower CO_2 emission factors for the process system compared to other coal chemical products and processes since they do not involve coal gasification reaction. In both methods to transform coal to oil, whether in the process or energy system, direct liquefaction has lower CO_2 emission factors as compared to indirect liquefaction. Because direct liquefaction can liquefy coal and synthesize liquid hydrocarbon fuel by catalytic hydrogenation under high temperatures and high-pressure conditions whereas indirect liquefaction will first gasify coal and then convert it into hydrocarbon fuel by the Fischer-Tropsch synthesis process. However, direct liquefaction requires higher quality coal and reaction and operating conditions. The product also contains a significant share of impurities, such as aromatic hydrocarbons, sulfur and nitrogen and has a low cetane number, which means it is more difficult to directly burn fuel in engines.

3.2. CO_2 emission of the coal chemical industry in China by product

The total CO_2 emission of different coal chemical products in China in 2015 is shown in Table 3. The total CO_2 emission of CCI in China in 2015 was 607 Mt (590–625 Mt), in which coal-to-ammonia was the largest contributor, accounting for 31.9% of total CO_2 emission, followed by coal-to-methanol (23.2%), coal-to-urea (16.9%) and coal-to-coke (15.9%). The results indicate that these four sub-sectors should be the highest priorities with regard to energy saving and CO_2 mitigation in China's coal chemical industry. These traditional CCPs are closely linked to other industries in China. Coal-to-ammonia and coal-to-urea provide nitrogen fertilizer for agriculture to meet the food demand of the large Chinese population. Coal-to-coke supplies coke for the iron and steel industry to support the demands of China's rapid development. Methanol is considered to be the center of a prosperous chemical industry network since it has always served as a fundamental raw material to produce other organic chemicals, such as dimethyl ether (DME) and acetic acid. Traditional CCI has undergone rapid development in China over the years [1] and it responsible for much (88.4%) of total CO_2 emission in 2015 due to the much higher output of traditional coal chemical products as compared to the modern coal chemical industry. However, the development of traditional CCI is basically saturated, whereas the modern CCI still has vast potential for development in the future. Therefore, the pattern of CO_2 emission of CCI may change significantly as time goes on.

Table 3
Total CO_2 emission of China's coal chemical industry in 2015 differentiated by product.

Coal chemical product	Process system (10^4 t)	Energy system (10^4 t)	Total (10^4 t)
Coal-to-coke	5359.79	4263.59	9623.38
Coal-to-ammonia	13675.01	5665.59	19340.60
Coal-to-urea	4242.66	6000.17	10242.82
Coke-oven gas-to-methanol	211.27	107.24	318.51
Coal-to-methanol	8421.27	5672.41	14093.68
Coal-to-olefin	2317.97	1413.59	3731.55
Methanol-to-olefin	0	788.02	788.02
Coal-to-ethylene glycol	426.93	641.46	1068.39
Coal-to-natural gas	657.21	230.65	887.86
Coal-to-oil (direct liquefaction)	260.53	96.86	357.39
Coal-to-oil (indirect liquefaction)	129.08	71.87	200.95
Total	35701.71	24951.44	60653.16

In the traditional CCI, coke-oven gas-to-methanol generates minimal CO_2 emission because coke-oven gas is a by-product of coking, which, incidentally, is used to synthesize methanol. The production of methanol transforming from coke oven gas is therefore not extensive. In the modern CCI, coal-to-olefin has the most significant CO_2 emission and is also one of the most mature modern coal chemical technologies. Due to the immaturity of coal-to-oil technology, only four coal-to-oil enterprises went into operation and had an unstable production status in 2015. Therefore, the production of coal-to-oil was only 1150 kt. The results also show the contributions of CO_2 emission from the process and energy systems are 58.8% and 41.2%, respectively. The CO_2 emission of the process system is higher because the products and processes, which are the main contributors, have higher CO_2 emission of the process system, excluding coal-to-urea.

3.3. Regional CO_2 emission of the coal chemical industry in China

The CO_2 emission of CCI in China has significant regional differences, as shown in Fig. 3 (see Tables S3 and S4 for more details). The bulk of CO_2 emission is distributed in northern China, where coal is relatively abundant. Shandong, Inner Mongolia and Shanxi are the three provinces that most contribute to CO_2 emission and cover one-third of the total CO_2 emission of the entire CCI, accounting for 12.3% (74.6 Mt), 11.3% (68.9 Mt) and 9.8% (59.6 Mt), respectively. Next, Henan, Shaanxi, Ningxia, Hebei, Xinjiang and Hubei, account for 9.5% (57.8 Mt), 7.9% (48 Mt), 5.5% (33.4 Mt), 5.1% (30.8 Mt), 4.5% (27.3 Mt) and 4.3% (26.2 Mt), respectively. Over 70% of CO_2 emission is from these ten provinces.

To further analyze the distribution characteristics of CO_2 emission of CCI, we assess the spatial distribution of the CO_2 emission of the four major coal chemical products, as shown in Fig. 4. The spatial distribution of the CO_2 emission of ammonia and urea indicates that the factors driving the carbon emission of CCI are not only coal reserves but also market demand for the products. The two provinces with the largest CO_2 emission of coal-to-ammonia and coal-to-urea, Shandong and Henan provinces, are also large agricultural provinces that consume large amounts of fertilizers. The total CO_2 emission of Shandong and Henan account for 15.7% (30.3 Mt) and 21.1% (21.6 Mt) of the CO_2 emission of coal-to-ammonia and coal-to-urea, respectively. Another

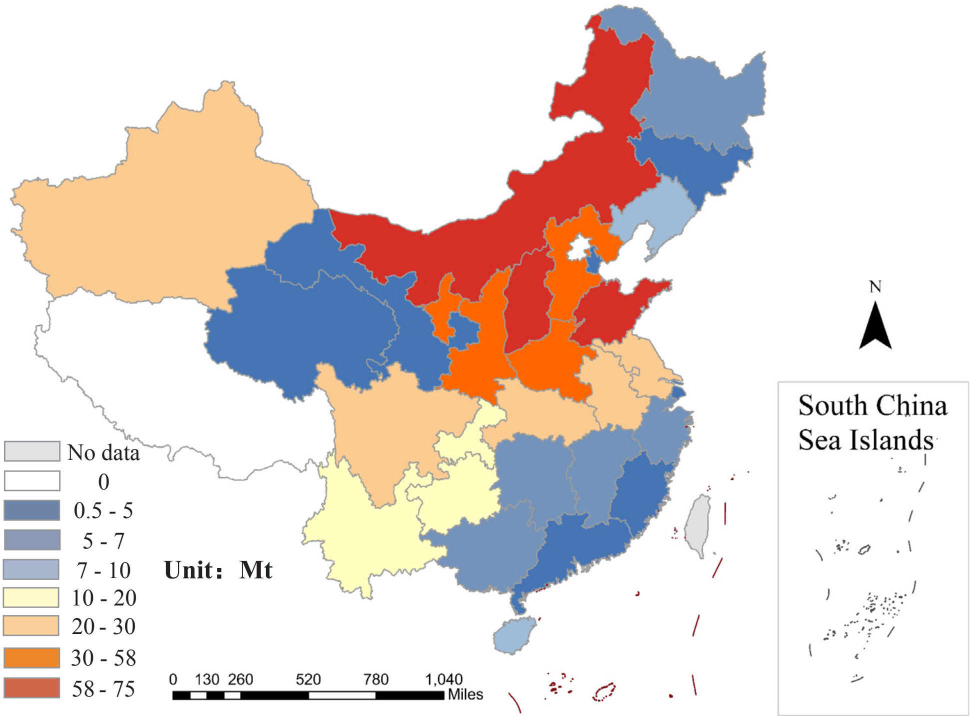

Fig. 3. Spatial distribution of CO_2 emission of CCI in China in 2015.

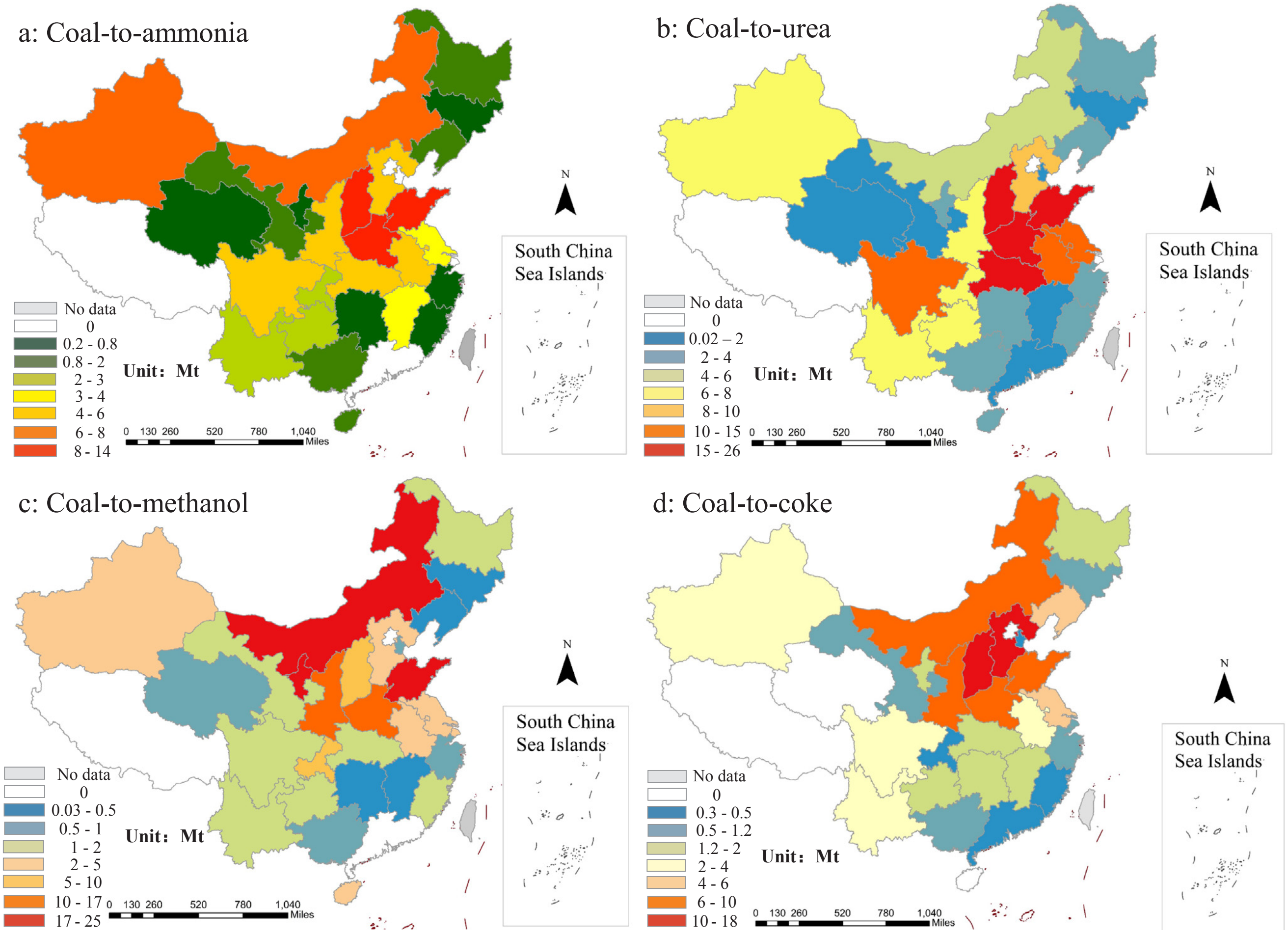

Fig. 4. Spatial distribution of CO_2 emission of the four major coal chemical products and processes in China in 2015.

Table 4
Comparison of CO_2 emission factors from previous research.

Product and process	Data sources	Emission factor (t CO_2/t product)
Coal-to-methanol	This study	4.26
	Qin et al., 2016 [25]	2.76
	Zhu et al., 2010 [34]	3.36
	Yi et al., 2015 [5]	2.60
Coal-to-ammonia	This study	4.44
	Zhou et al., 2010 [6]	4.58
	Zhu et al., 2010 [34]	4.65
	Yi et al., 2015 [5]	3.30
Coal-to-olefin	This study	10.50
	Ren and Patel, 2009 [35]	[8,11]
	Gao et al., 2018 [21]	11.00
	Yi et al., 2015 [5]	9.30
Coal-to-coke	This study	0.21
	Yi et al., 2015 [5]	0.20
Coal-to-oil (indirect liquefaction)	This study	7.52
	Zhou et al., 2014 [36]	6.90
Coal-to-oil (direct liquefaction)	This study	4.02
	Yi et al., 2015[5]	3.50
Coal-to-natural gas	This study	6.66
	Li et al., 2014 [24]	5.92
	Liu et al., 2017 (Liaoning) [37]	6.69
	Liu et al., 2017 (Inner Mongolia) [37]	6.97
	Liu et al., 2017 (Xinjiang) [37]	7.00

example is Shanxi, the largest coke producer, accounts for 18.4% (17.7 Mt) of the CO_2 emission of coal-to-coke, which is mainly used in steelmaking. Inner Mongolia, Shandong, Ningxia and Shaanxi are the largest contributors to the CO_2 emission of coal-to-methanol, accounting for 17.5% (24.7 Mt), 15.4% (21.7 Mt), 12.5% (17.6Mt), and 10.7% (15 Mt), respectively. Inner Mongolia, Ningxia and Shaanxi are all rich in coal resource and thus provides abundant raw material.

3.4. Results comparison with earlier studies

We compare our CO_2 emission factors with current research, as shown in Table 4. The emission factors in this study are consistent with those published in previous studies, except for coal-to-methanol. When analyzing the calculation methods described in earlier papers, we find probable reasons. First, the process data in Qin's research [25] are based on ASPEN Plus software simulation and differ from actual production data. Based on the conservation of carbon element, 33.4% carbon element in the raw material enters into the product in Qin's research [25], which is relatively similar to the 32.99% and 34.94% of the enterprises surveyed in this study. However, only 48% carbon element in Qin's study [25] is emitted in the form of CO_2, which is quite different from 63% and 64% in our study. The main reason for this difference is that the emission data come from software model simulations and no further treatment of the process exhaust gas is taken into consideration. However, carbon containing organic substances such as CO and CH_4 in the exhaust gas will be partly converted to CO_2 and then emitted into the atmosphere, considering part of the exhaust gas will be burned through the high-pressure torch in the actual process. Second, the energy consumption data of the reference [33] cited in Qin's research [25] only cover the energy consumption of methanol production facilities without considering the consumption of public facilities, such as desalinated water stations, circulating water stations and air separation stations. Also, the emission factors in Yi's study [5] are lower than ours but it is difficult to determine why since the review paper does not provide any detailed data sources. We infer that the main reason may be a difference in system boundaries.

4. Discussion

4.1. Scenario analysis of CO_2 emission of modern CCI in China in 2020

Although modern CCI only contributed a small portion of total CO_2 emission of CCI in 2015, it has immense potential for growth. The development of modern CCI could significantly impact CO_2 emission. Furthermore, given the large amount of carbon emission of modern coal chemical processes, technology is likely to be used to reduce the footprint. Carbon capture, utilization and storage (CCUS) encompass methods and technologies to remove CO_2 from the flue gas and atmosphere, followed by CO_2 recycling for use and the determination of safe and permanent storage options—an emission abatement option with great potential. CCUS has been used in demonstration projects in China, including a coal-fired electricity generation plant. As part of the survey of coal chemical enterprises, we also found a CCUS demonstration project that recycles the CO_2.

In order to figure out whether the development of modern CCI will have a significant impact on CO_2 emission in the future and the effect of CCUS technology on the carbon emission of modern CCI, we conduct scenario analysis of CO_2 emission of modern CCI in China in 2020. CCUS may be used in a gasifier, as well as in a thermal power plant. Therefore, with CCUS, both the process and energy systems of CCI have the potential to reduce the CO_2 emission. Nevertheless, as compared to thermal power plants, CCUS applied in gasifiers entails a significantly lower cost. Owing to the characteristics of the technological process, the CO_2 concentration produced by the CCI is much higher than that of the flue gas of power plants and its capture cost is much lower than that of power plants. Therefore, we may reasonably assume that the technology will be promoted first in the coal chemical process system. We set up three scenarios based on the CCUS coverage. In the baseline scenario, neither the process system nor the energy system applies CCUS. In scenario 1, only the process system applies CCUS. In scenario 2, both the process sand the energy systems apply CCUS. We consider four major modern coal chemical products: coal-to-oil, coal-to-natural gas, coal-to-olefin, and coal-to-ethylene glycol. The production data of these products in 2020 are taken from government report [4] and the literature [38]. The capture efficiency data of CCUS comes from the literature [39].

The results of the scenario analysis are illustrated in Fig. 5 (see Tables S5 for detailed data). In the baseline scenario, according to government planning for modern CCI in 2020, if there is no CCUS, the CO_2 emission could be as high as 416.52 million tonnes which is 6.67 times higher than in 2015. Considering that traditional CCI has little development potential, the CO_2 emission proportion of modern CCI would increase significantly by 2020. In scenario 1, when CCUS is only applied to the process system, the CO_2 emission could be reduced by 198.31 million tonnes. In scenario 2, when CCUS is applied to both the process and energy systems simultaneously, the CO_2 emission could be reduced by 317.98 million tonnes, thus cutting the CO_2 emission by 76%. It is therefore possible to conclude that government planning for modern CCI would have a significant impact on carbon emission and that CCUS could significantly reduce the CO_2 emission. Otherwise, it is estimated that the contribution of the CO_2 emission of modern CCI to the entire CCI will increase from 11.6% in 2015 to 43.7% in 2020 if the traditional CCI CO_2 emission remains unchanged.

4.2. High CO_2 emission price of CCI on account of China's energy reserve structure

The development of CCI in China results from the special energy reserve structure, namely, abundant coal resource and relatively scarce oil and natural gas reserves. However, as compared to transforming oil

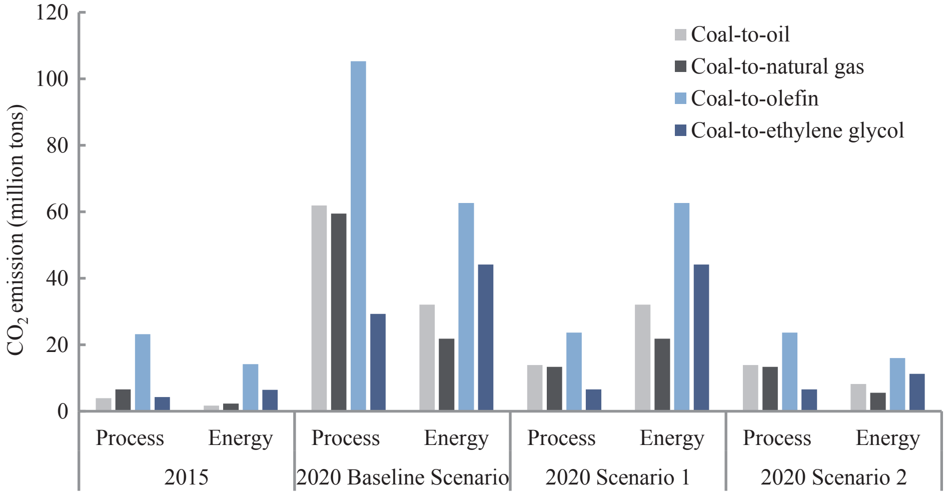

Fig. 5. CO_2 emission of modern CCI in China in 2020.

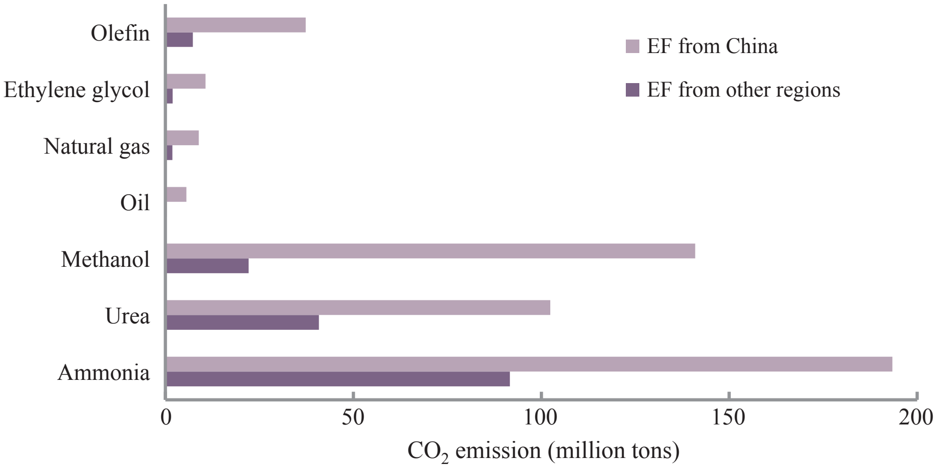

Fig. 6. Comparison of current CO_2 emission of CCI in China with hypothetical emission of alternative sourcing pathways (oil and natural gas instead of coal) in reference year 2015.

and natural gas to chemicals, transforming coal to chemicals has much higher CO_2 emission factors due to chemical process characteristics. Transforming coal to oil or natural gas also leads to higher CO_2 emission as compared to directly exploiting oil or natural gas. In addition, coal-fired thermal power dominates the Chinese grid and contributes to higher CO_2 emission of the energy system. Considering all the factors, the high CO_2 emission of China's CCI is the consequence of the energy reserve structure. In order to quantify the superfluous CO_2 emission of CCI caused by China's energy reserve structure, we replace the CO_2 emission factors of coal-based chemical products in China with those of oil-based or natural gas-based products from other data sources (see Tables S6 for more details). As shown in Fig. 6, the results indicate that China could hypothetically reduce the CO_2 emission by 333.24 million tonnes (namely 66.7%) if the chemicals were produced by alternative production pathways relying on oil and natural gas rather than coal chemical processes.

The two main solutions to solve the problem of the uneven distribution of resources between countries are international trade and alternative resources. The results in Fig. 6 indicate that there is huge potential to reduce the CO_2 emission of China's CCI through international trade. However, in the long term, with the development of global economy, non-renewable resources such as oil and natural gas will become increasingly scarce. Biomass-based fuel could be another alternative for coal chemical products in the future. For example, Brazil has been developed bioethanol industry since the 1970s due to the oil crisis in an effort to decrease its dependence on imported oil [40]. Biofuel is regarded as a promising and low carbon emission energy because it is generated by photosynthesis and the emitted CO_2 emission is essentially from the CO_2 absorbed by plants. The Chinese government can learn from other countries' experiences in developing biofuels to set up a low-carbon development path that considers China's resources and agricultural conditions.

4.3. Policy implication

According to previous research [41] and the results of this study, CO_2 emission of the coal chemical industry in 2015 was 607 million tonnes (Mt), accounting for approximately 5.71% of China's total CO_2 emission. The figure is even higher than the total annual CO_2 emission of a country such as Canada (555 Mt) or Brazil (486 Mt). Quantifying the emission of the coal chemical industry is therefore critical to understand the global carbon budget and it is therefore critical for the government control the CO_2 emission of CCI for the government. Considering the much higher CO_2 emission factors of coal-based chemicals as compared to oil-based and natural gas-based options, the government could foster the import of natural gas and oil by tariff concessions to make up for resource endowment shortcomings. Moreover, under the premise of sufficient food supply, biomass-based fuel ethanol remains a good alternative for coal-based fuels considering its potential to alleviate environmental impacts [42].

As for traditional CCI that has developed so many years, the government could encourage these enterprises to replace their backward production technologies and equipment by more efficient alternatives. For instance, the survey conducted for this study reveal that some coal chemical processes, such as gasification, are exothermic reactions, and waste heat recovery device could be installed to reduce fuel consumption and CO_2 emission. Washed coal, which has a lower ash content, could replace raw coal to improve burning efficiency. As for modern CCI, which is developing rapidly, the concept of energy conservation and emission reduction could be reflected in the design, build and operation of coal chemical projects. Currently, most modern coal chemical enterprises are located in large industrial zones with abundant coal resources and are located quite close to each another. The local government could fully develop the industrial cluster effect of the coal chemical zones and achieve the scale effects through the efficient centralization of the heating and electricity supply. Furthermore, the concentration of industrial activity in these areas creates an opportunity to develop industrial symbiosis in energy and materials exchange between plants, which could help plants improve energy efficiency and reduce carbon emission. For example, Yi et al. found that the coke oven gas from coking plants reacts with the recycled CO_2 separated from the CO_2-rich exhaust gas to produce syngas for synthetic natural gas production [43]. It can significantly improve the hydrogen utilization efficiency in coke oven gas, which not only increases SNG production and thus enhances energy efficiency, but also reduces the CO_2 emission.

According to the spatial distribution characteristics of the CO_2 emission of CCI, CCI is being developed in northern China with a higher proportion of thermal power generation, so the embedded carbon emission is larger. The government could encourage the use of clean energy, such as wind and solar energy, based on the local conditions. For example, Xinjiang, Ningxia and Inner Mongolia are endowed with a rich solar radiation resource that have tremendous potential for solar power generation. In addition to the high carbon emission, the CCI emits a large amount of waste gas, waste residue and wastewater. The wastewater that is produced, and especially the wastewater with high concentration of salt and refractory organics, is very difficult to manage. The emissions of these pollutants can reduce the local environmental quality, thereby affecting human and ecological health. There are also underdeveloped provinces, such as Xinjiang, Ningxia and Inner Mongolia, in which many large-scale coal chemical enterprises are located. These regions are prone to pursuing economic development excessively and ignoring environmental. Xinjiang, Ningxia and Inner Mongolia in particular are also faced with fragile ecological environment. Therefore, the government could strictly monitor these coal chemical enterprises to avoid unrecoverable ecological damage. Meanwhile, these coal-rich provinces provide abundant chemical materials, liquid fuels and SNG to other regions to support their own development. For example, SNG for municipal heating could be a cleaner alternative than coal to mitigate of haze pollution in metropolitan areas [8]. Coal-based SNG is produced in Xinjiang and Inner Mongolia and then transported to developed cities as clean energy, which means that the pollution is transferred to these developing regions. We suggest implementing industry-wide ecological compensation to balance ecological protection and economic development: the urban areas that benefit from the coal-based clean energy should have to make a financial contribution to support environmental protection in coal chemical production regions and the implementation of more advanced environmental protection facilities within the coal chemical enterprises.

5. Conclusion

This study provides the CO_2 emission factors of coal chemical products produced in China based on firsthand data from twenty-three coal chemical enterprises that can provide data for subsequent carbon accounting researches. We then extrapolate the total CO_2 emission from China's coal chemical industry: 607 Mt (590–625 Mt) for reference year 2015. China's coal chemical industry has become one of the largest industrial CO_2 emission sectors. The spatial pattern of CO_2 emission from the coal chemical industry implies that the industry is strongly influenced by coal resource, and the majority of the CO_2 emission is distributed in northern China, where coal is relatively abundant. In addition, the spatial distribution of CO_2 emission of coal-based ammonia and urea production indicates that market demand for chemicals is also an important driving factor. The two provinces with the largest CO_2 emission of coal-to-ammonia and coal-to-urea, Shandong and Henan, are also large agricultural provinces that consume large amounts of fertilizers. Shandong, Inner Mongolia and Shanxi are the top three provinces which contribute the largest amount of CO_2, covering one-third of the total CO_2 emission of the coal chemical industry. For the underdeveloped provinces in which many large-scale coal chemical enterprises are located, the government strictly monitor these coal chemical enterprises to avoid pursuing economic growth blindly and ignoring environmental problems. The results also show that the traditional coal chemical industry contributes to 88.4% of the total CO_2 emission due to the higher output of coal chemical products as compared to the modern coal chemical industry. However, modern CCI has immense potential for growth. According to the government plan for the modern coal chemical industry in 2020, with no carbon capture, utilization and storage, the CO_2 emission could be as high as 416.52 million tonnes: 6.67 times higher than in 2015. Scenarios with carbon capture, utilization and storage could reduce CO_2 emission by 317.98 Mt. This study provides valuable data to support the development of CO_2 mitigation policies for the coal chemical industry that consider the local realities.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.apenergy.2018.12.022.

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