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Life-cycle environmental burdens of ethylene production in the context of China's chemical feedstock transition from naphtha to coal and shale gas by-product of ethane

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ABSTRACT

China is experiencing an ethylene-feedstock transition from naphtha to cheap coal and ethane by-product of shale gas. This transition leads to the variation in the environmental burdens of ethylene production. Here, we compared the life-cycle environmental loads of ethylene, produced by four typical routes—naphtha to ethylene (OTE), ethane to ethylene (ETE), coal-based methanol to ethylene (CMTE), and bioethanol to ethylene (BETE). Global midpoint environmental impacts (with 12 indicators) and China-contextualized Energy Conservation and Emission Reduction (ECER) index were used. We found that the trade-off across the 12 environmental dimensions impedes directly comparing the environmental sustainability of the four ethylene routes. The emerging ethane-fed ETE route, as an example, generates low climate change loads (GWP) but high abiotic resource depletion potentials (ADP). China's indigenous ECER index, addressing this trading-off issue, shows the highest environmental burdens of the coal-fed CMTE route, followed by the BETE, ETE, and OTE routes. Raw material consumption dominates 58–85% environmental burdens of the four ethylene routes. Referring to the 2018 baseline, replacing the coal-fed CMTE route with the ethane-fed ETE would reduce the environmental load per tonne of ethylene product by 2–25% in 2030 and 6–42% in 2050. However, the total environmental loads of China's ethylene sector would still increase by 1–44% and 6–68% due to the continued industrial expansion. Given ethylene as the primary chemical material, our findings provide policymakers with reference to promote the environmental sustainability of chemical manufacturing sector.

1. Introduction

Ethylene, an essential primary chemical material, dominates >75% of global petrochemical production (Cngold.org, 2019; CBMF, 2021). Thus, its environmental impacts attract great attention (Gao et al., 2019; Cao et al., 2021). China is the world's second-largest ethylene producer, with production exceeding 30 million metric tons (Mt) in 2020 and expected to be up to 42.7 Mt. by 2030 (Chen et al., 2018). The energy intensity of China's ethylene product was 800 kgce t^{-1} (kilograms of standard coal equivalent/ton) in 2019, and its total energy is responsible for 0.67% of national energy consumption (Energy Foundation, 2021). According to the 14th Five-Year Plan, China needs to reduce its energy (carbon) intensity by 13.5(18)% by 2025, referring to the 2020 level (IEA, 2021). Therefore, in the context of climate change, evaluating and reducing carbon emission from manufacturing industry (e.g., the ethylene sector) is crucial for China's double carbon goals (Peng et al., 2022).

Ethylene is produced mainly by four routes, i.e., naphtha-fed ethylene (OTE), ethane-fed ethylene (ETE), coal-fed ethylene (CMTE), and bioethanol-fed ethylene (BETE) routes. Global (except China) ethylene production is dominated by the OTE route (sharing 70%) and ETE route (25%; Hu, 2016). Particularly, the U.S. shale-gas revolution that occurred in the 2000s is systemically changing the composite of global ethylene feedstock. This change attributes to the explosive growth in ethane production—as a cheap light alkane by-product of shale gas (Zhang et al., 2018). For example, the capacity share of ethane-based ETE route in the U.S. grew from 68% in 2015 (Statista, 2017) to a projected over 80% in 2020 (CPCIF, 2019b). China's ethylene capacity,

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unlike the U.S., is dominated by the naphtha-fed OTE route (sharing 74%) and the coal-fed CMTE route (20%) in 2020 (Huaon, 2022). Coal-fed CMTE route continues to grow in China due to the low cost of feedstock (Xiang et al., 2014a), but with high carbon intensity. Besides, China has the world's largest recoverable shale gas resources (32 trillion m^3), nearly twice that of the U.S. (EIA, 2015). China has been accelerating its shale-gas exploration to replace coal for energy system decarbonization, with ethane production growing from 80 kt (Kt) in 2015 to 1.6 Mt. in 2020 (Chyxx, 2021). Therefore, the newly emerging ETE route with ethane as feedstock keeps soaring and reaches up to 2% of China's ethylene capacity in 2020 (Huaon, 2022). This feedstock change influences the overall environmental impacts of the ethylene industry.

The environmental loads of olefin (including ethylene) production varies across routes. For example, Yang and You (2017), by life-cycle analysis, found that the ETE route was less water intensive (202%), but more carbon intensive (27%), referring to the conventional naphtha-fed OTE route. Chen et al. (2017) demonstrated that natural gas-based olefins were 60% higher eco-efficient than the coal- and oil-fed routes. Besides, the ethylene produced from shale gas via coupled methane oxidation (OCM) processes is more profitable than that of the MTO process (Ortiz-Espinoza et al., 2017). Yang et al. (2018) conducted a comparative analysis of three pathways based on ethane-rich shale gas, corn stover, and corn kernels, and showed that the shale gas-based pathway showed the best economic performance, but it resulted in the highest net ethylene GHG emissions.

For coal, oil, and bioethanol-fed ethylene routes, Zhao et al. (2014) and Chen et al. (2018) showed that coal-based routes are three and eight times more carbon intensive than oil-based route. The life-cycle assessment shows the climate advantage of the bioethanol-fed ethylene route over that of the petrochemicals (DME) (Alonso-Farinas et al., 2018). However, market penetration of the bioethanol-fed route is limited due to low profitability (e.g., Hong et al., 2014; Yang et al., 2018, and Alonso-Farinas et al., 2018). Also, Keller et al. (2020) and Young et al. (2020) quantify the resource and environmental load of olefin production in Germany and the USA.

Although the issue of environmental sustainability of ethylene produced by multiple routes has been partially investigated by researchers in the current research literature. However, the context of the ongoing rapid feedstock transition from naphtha to coal and ethane in China and the quantification of the total environmental load of the ethylene industry are not considered at the national level. Related literature fails to provide a clear answer. The contents of this study, informing the transition of chemical feedstocks in China, are exactly where the existing research literature falls short. It not only addresses the quantification of the overall environmental impact generated by ethylene in various countries and regions around the world to provide a reference but also addresses the choice of sustainable pathways for China's policymakers.

Therefore, we investigated the followings in this research: (1) Quantitatively compare the life-cycle environmental burdens of 1 t ethylene produced by four different ethylene production routes (i.e., naphtha-fed OTE, ethane-fed ETE, coal-fed CMTE, and bioethanol-fed BETE routes); (2) perform sensitivity analysis to identify the key factors influencing the magnitude of environmental loads; (3) evaluate the total environmental burdens of China's ethylene industry in the 2018 baseline, and predict the total burdens in the target years 2030 and 2050 under predefined scenarios of ethylene-feedstock transitions.

2. Data and methodology

The life cycle assessment (LCA) approach, widely used such as by Zhuang et al. (2023) and Mazzetto et al. (2023), was applied here to quantify the environmental burdens of ethylene product. According to ISO 14040 (2006), the LCA method consists of four stages, i.e., functional unit and system boundary definition, inventory analysis, impact assessments, and result interpretations. JRC-IEA (2010) provides two modeling approaches of attributional LCA and consequential LCA. The former describes the environmental and physical flows to-and-from the production system and associated subsystems, while the latter aims to quantify how the associated environmental and physical flows are affected by decision-making. We referenced to Finnveden et al. (2009) and Ekvall et al. (2016) and selected the attributional approach to develop the LCA models in this study with impacts attributing to the functional unit (Weidema et al., 2018).

2.1. *Objective and scope definition*

The objective of this LCA analysis is to quantitatively compare the environmental loads of the four ethylene production routes (ETE, OTE, CMTE and BETE). The functional unit was defined as one metric ton of ethylene product in 99.9% purity. The system boundary is the cradle-to-gate, including raw material extraction and ethylene production. In particular, we choose data from typical domestic process companies as the reality data for building LCA models, and for the feedstocks used in upstream production (naphtha, ethane, and coal, etc.), we connected to the local Chinese CLCD database (Yue et al., 2016); and for the missing data in the CLCD database, we selected the ecoinvent database as alternative where the upstream full inventory data of feedstocks are available (e.g., Frischknecht et al., 2005; Wernet et al., 2016) to ensure the full "cradle-to-gate" scope of our analysis. Fig. 1 shows the system boundary.

The inputs consider the consumption of all raw materials, energy, electricity, steam, water, and auxiliary chemicals in each production process and sub-processes. The output includes ethylene products and propylene co-product. The mass method was used to allocate the quantified environmental loads between ethylene and propylene co-product. Notably, this study focuses on the deficiency in environmental burdens of one-tonne ethylene produced by the four routes. Therefore, the ecological impacts of ethylene applications, end-of-life waste disposal, plant facility construction, and equipment maintenance were excluded from the evaluation boundary.

2.1.1. *Production routes and case factories*

(1) Ethylene to ethane route (ETE)

The system boundary with the main processes of the ETE production route is shown in Fig. 1a. The specific process uses CNPC's own-developed ethane-to-ethylene technology by high-temperature steam cracking. The cracking furnace is HQF-IV, and the cracked products are further separated to produce ethylene by pre-destination pre-hydrogenation technology.

The case plant for the ETE route is selected from Lanzhou Petrochemical Co of PetroChina Gas. The project was built in 2018 and is located in Yulin, Shaanxi Province. The annual ethane processing capacity of the factory is 1.05 Mt. to produce 800 Kt of ethylene product. Specifically, ethane feedstock is steam-cracked to prepare ethylene, which is then polymerized to prepare olefins. The products include C3 fraction and by-products such as recombinant fraction and fuel oil. The feedstock inputs include ethane feedstock, electricity, steam, demineralized water, and auxiliary materials (i.e., 20% wt of sodium hydroxide and sulphuric acid).

(2) Naphtha to ethylene route (OTE)

The system boundary and main processes of the OTE route are shown in Fig. 1b. The specific ethylene production process is from naphtha by a typical steam cracking. Steam cracking facilities include an ethylene steam thermal cracking unit, a dry gas recovery unit, a waste alkali oxidation unit, a variable adsorption-hydrogen production unit, and an ethylene cryogenic storage tank. The case factory for the OTE route is Hengli Petrochemicals Co, located in Dalian, Liaoning Province. The factory was built in 2018, with a production capacity of about 1.5 Mt.

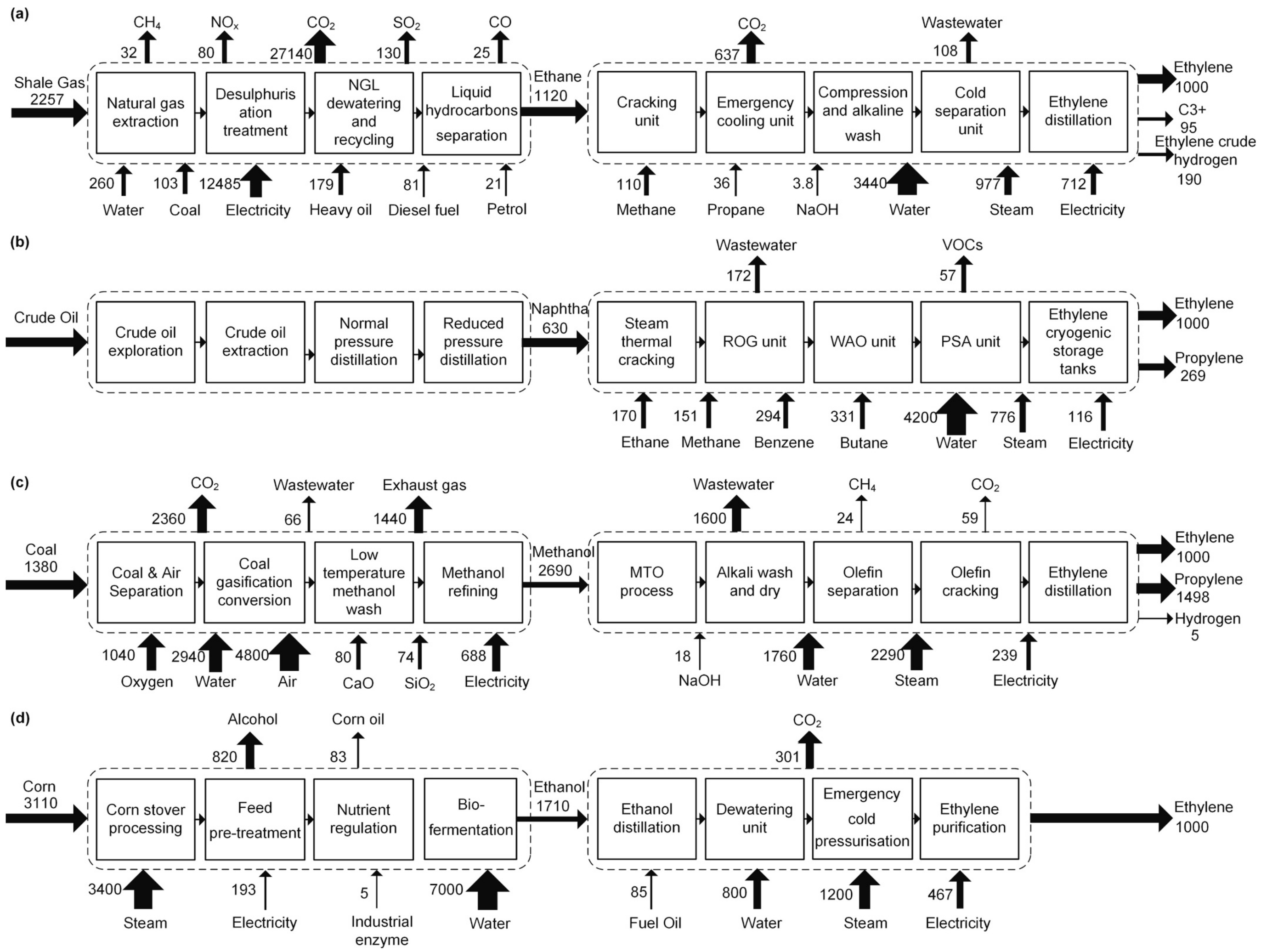

Fig. 1. System boundaries for four ethylene production routes. **(a)** Natural gas-based ethane to ethylene (ETE). **(b)** Naphtha to ethylene (OTE). **(c)** Coal-based methanol to ethylene (CMTE). **(d)** Ethylene from bio-based ethanol (BETE). The unit of natural gas is m^3 and that of electricity is kWh. The units of industrial enzymes are liters. Units of other materials are kilograms.

yr^{-1}. The significant inputs of the project include naphtha, mixed C4 fraction, ethane, methane, fresh water, steam, electricity, and auxiliary materials (i.e., propane and benzene).

(3) Coal-based methanol to ethylene route (CMTE)

The system boundary of the CMTE route is shown in Fig. 1c. The specific process includes the preparation of pulverized coal from raw coal and generating crude gas via air separation. The natural gas is then converted to hydrogen and carbon monoxide after removing the acid gas. Next, the low-temperature methanol washing process purifies the gas, which is then transported to the methanol synthesis unit to produce crude methanol. By distillation, the crude methanol generates MTO-grade methanol.

The case plant for the CMTE route was selected from the project joint developed by China Power Investment Co and Total Group. This case factory, located in the coal-rich Inner Mongolia Autonomous Region, was built in 2016, with an annual ethylene production capacity of 350 Kt. The inputs for this factory include coal feedstock, electricity, steam, fresh water, air, and auxiliary materials of 40% wt sodium hydroxide.

(4) Bio-ethanol to ethylene route (BETE)

Fig. 1d shows the system boundary and main processes of the BETE route. These processes include fermentation to ethanol and dehydration and pressurization of ethanol to ethylene. Firstly, the corn stover or kernels are treated by bio-fermentation technology to produce ethanol. Ethanol dehydration follows this to ethylene, where the bioethanol is processed through a distillation and dehydration unit. Finally, olefins are produced by quenching and pressurizing to produce ethylene products. The case factory for the BETE route was selected from a corn ethanol plant in Anhui province, built in 2005. The plant inputs include corn straw, glucose, 93% wt concentrated sulphuric acid, electricity, and water.

2.2. Inventory analysis

We applied the eFootprint online platform to construct the LCA model. The platform is embedded with the CLCD database focusing on the local Chinese industrial system. Besides, eFootprint is compatible with the Ecoinvent as a supplementary database (Liu et al., 2010). The platform is popular in China and has been used for various applications in previous studies (Lv et al., 2021; Zhao et al., 2021).

We obtained the real-world foreground data of the four ethylene routes from the publicly available official environmental impact assessment reports for chemical companies. Literature and company research data were also reviewed as a supplement. Background data on feedstock (coal, naphtha, natural gas, corn) and energy (electricity, industrial water, steam) for the life-cycle models of the four ethylene production routes were obtained from the CLCD and Ecoinvent databases. The oil, natural gas, and coal extraction were linked to the China context CLCD database. For the feedstock to produce ethanol in the BETE route, maize production inventory was linked to the Ecoinvent database to represent the average status of China's market. We developed an LCA model for the four ethylene production routes with data handling principles as Qian et al. (2022). Table 1 gives the details.

2.3. Impact assessment methods

The environmental impacts assessment includes two methods of midpoint and endpoint. The former focuses on the varied environmental impacts before the endpoint of environmental impact is reached. The midpoint evaluation method has low uncertainty and produces more accurate results than the endpoint method (Huijbregts et al., 2017). Thus, we selected the 12 midpoint indicators to compare the environmental loads of the four ethylene production routes. However, trade-offs exist across these midpoint indicators, thus making it difficult to compare the four processes' environmental performance directly. Therefore, based on the midpoint indicator, we further calculated the China-specified Energy Conservation and Emission Reduction (ECER) metric to compare the comprehensive environmental performance of the four ethylene production routes by normalized ECER results (Wang et al., 2013).

(1) Midpoint assessment

The midpoint approach includes twelve environmental impacts, i.e., climate change (GWP, $kgCO_2e$), primary energy demand (PED, MJ), abiotic depletion potential (ADP, kgSb-e), water depletion (WU, kg), acidification (AP, $kgSO_2e$), eutrophication potential (EP, $kgPO_4^{3-}e$), respirable inorganic matter (RI, $kgPM_{2.5}e$), ozone depletion (ODP, kgCFC-11e), photochemical ozone synthesis (POFP, kgNMVOCe), ionizing radiation-human health (IRP, kgU235e), eco-toxicity (ET, CTUe), and human toxicity-carcinogenesis (HT-cancer, CTUh).

The eFootprint online modeling system generated these indicators. The GWP parameters were derived from "5^{th} assessment report" from IPCC (2014); the ADP, AP, EP, and ODP environmental impacts were from CML2002; the RI impacts from IMPACT2002+; and the POFP impact indicators from the ReCiPe method. PED indicates the total consumed calories of primary energy that covers coal, oil, and natural gas. WU metric tells the consumption of water resources. IRP indicates the amount of ionizing radiation from uranium, ruthenium, radium, manganese, etc. ET means short- and long-term emissions of toluene, xylene, mercury, lead, etc. HT-cancer indicates the produced volume of carcinogenic substances such as benzo(*a*)pyrene and PCBs.

(2) China's ECER Index

The ECER index is based on the LCA methodology and in accordance with the energy saving and emission reduction policy objectives, which allows for a quantitative, comprehensive and integrated evaluation of the four ethylene production processes and the drawing of clear conclusions. The ECER composite index includes the main binding indicators specified in the 13th Five-Year Plan for National Economic and Social Development, as shown in Table S2. This includes seven categories of indicators, namely PED, IWU, CO_2, SO_2, COD, NO_X and NH_3-N.

China's ECER index allows a comparison of the environmental performance of the four ethylene production routes rather than highlighting a particular environmental dimension in isolation. Thus ECER effectively avoids the tradeoff issue and is calculated as follows (Wang et al., 2013).

Table 1
Inventory data of the four process routes for the production per 1 t of ethylene.

Parameter	Name	Unit	ETE[a]	OTE[b]	CMTE[c]	BETE[d]
Input	Ethane	tonne	1.12	0.17	–	–
Input	Methane	kg	110	151	–	–
Input	Propane	kg	36.2	41.3	2687.8	–
Input	Methanol	kg	–	–	–	–
Input	Dimethyl disulfide	g	170	–	72.6	–
Input	NaOH	kg	3.8	–	18.7	0.6
Input	CO	kg	0.27	–	–	–
Input	Sulphuric acid(98% wt)	kg	0.44	–	–	–
Input	Hydrogen	kg	86.2	–	–	–
Input	Instrumentation Air	m^3	39.5	–	4.8 (t)	–
Input	Nitrogen	m^3	5.33	–	–	–
Input	Natural gas	m^3	2257	–	–	–
Input	Coal	kg	103	–	1380	–
Input	Petrol	kg	21	–	–	–
Input	Diesel fuel	kg	81	–	–	–
Input	Heavy oil	kg	179	–	–	–
Input	Fuel gas	m^3	65.5	–	–	–
Input	Naphtha	tonne	–	0.63	–	–
Input	C4	kg	–	129	–	–
Input	Butane	kg	–	331	–	–
Input	Benzene	kg	–	294	–	–
Input	Purification gas	tonne	–	–	1.1	–
Input	Oxygen	tonne	–	–	1.04	–
Input	CaO	kg	–	–	80.5	–
Input	SiO_2	kg	–	–	74.3	–
Input	Hydrochloric acid	g	–	–	0.82	–
Input	Corn	tonne	–	–	–	3.11
Input	Liquefaction enzymes	L	–	–	–	1.62
Input	Glycolytic enzymes	L	–	–	–	2.4
Input	Yeasts	kg	–	–	–	0.1
Input	Sulphuric acid	kg	–	–	–	1.5
Input	$CaCl_2$	kg	–	–	–	0.5
Input	Ethanol	tonne	–	–	–	1.71
Input	Fuel oil	kg	–	–	–	85
Input	Super high pressure Steam	kg	742	–	–	–
Input	High pressure steam	kg	–	776	–	–
Input	Medium pressure steam	kg	235	–	1213.4	1200
Input	Low pressure steam	kg	–	–	2713.8	3400
Input	Electricity	kWh	712	116	927	563
Input	Desalted water	tonne	3.7	4.2	4.7	7.8
Output	Ethylene	tonne	1	1	1	1
Output	BOD_5	g	60.3	–	88.7	–
Output	COD_{Cr}	g	229	–	371.8	–
Output	TDS	g	7380	–	546.7	–
Output	NO_X	kg	81	0.48	–	–
Output	CO	kg	25.5	0.28	–	–
Output	SO_2	kg	130.2	0.06	–	–
Output	VOCS	g	98	56.5	–	–
Output	CO_2	kg	637	1.39	2419.5	300.8
Output	CH_4	kg	32.6	–	23.93	–
Output	Wastewater	kg	108	172	1666	–
Output	Propylene	tonne	–	269.2	1498	–
Output	C3+	kg	94.6	–		–
Output	Fuel Oil	kg	4	–	60	–
Output	Hydrogen	kg	0.37	–	5.6	–
Output	Liquefied Petroleum Gas	kg	–	–	42.4	–
Output	C5	kg	48	–	51.8	–
Output	Gasoline	kg	–	–	83	–
Output	Ethylene crude hydrogen	kg	190	–	–	–
Output	Mixed C4	kg	35	–	–	–

[a] Original data were obtained from the Environmental Impact Assessment Report of the CNPC Lanzhou Petrochemical Ethane to Ethylene Project and the publicly available environmental impact assessment report of Jiangsu Lianyungang Petrochemical Co.

[b] Original data were obtained from the published Environmental Impact Assessment Report of Hengli Petrochemical (Dalian) Chemical Co.

[c] Original data were from the published Environmental Impact Assessment Report of the joint venture project between CLP and Total.

[d] Original data were from the published Environmental Impact Assessment Report of the biomass ethanol project in Anhui Province. Follow the cut-off rule and ignore the environmental impact of complex chemicals with a mass <1% of the total material input.

$$ECER = \sum_{i=1}^{7}\left[\frac{A_i}{(T_i \times N_i)}\right] \quad (1)$$

where A_i represents the life-cycle environmental impact i per tonne of ethylene product (i = 1–7 for PED (MJ), IWU (kg) and CO_2 (kg), SO_2 (kg), COD (kg), NO_X (kg) and NH_3-N (kg)), which were quantified by the eFootprint online system. T_i represents China's energy saving and emission reduction target i in the latest Five-Year Plan periods. N_i (tonnes) represents the 2016 baseline of China's environmental loads i. T_i and N_i parameters were built-in the eFootprint system, see Table S2 for specific values. Wang et al. (2013) give the detail on the ECER methodology.

2.4. Uncertainty and sensitivity analysis

A good assessment of uncertainties is important for the identification of key substances in the production process in the different production routes of ethylene LCA (Groen and Heijungs, 2017). Uncertainties of our life-cycle models were sourced from the foreground and background data. The former represents the variations in the input-output inventory of each case factory for the four ethylene production routes. The latter, by contrast, represents uncertainty in the background Ecoinvent and CLCD databases (Bamber et al., 2020). We performed Monte Carlo simulations to quantify uncertainties of midpoint indicators per tonne ethylene product.

The four ethylene production routes involve various input and output materials. The variation of input generated different impacts on the varied environmental outputs. Sensitivity analysis, therefore, was conducted to identify the critical input variables influencing the outcomes of the LCA models (Huang et al., 2012). Specifically, the target input inventory parameters were set to vary by ±5% and ± 10% to examine the impacts of different input quantities on the output of each environmental burden. The results of the sensitivity analysis are presented in Section 3.3.

2.5. Scenario analysis

China's feedstock for the ethylene industry is transitioning from naphtha (OTE route) to coal (CMTE route), ethane (ETE route), and bioethanol (BETE route). We conducted the scenario analysis to assess the overall environmental loads of China's ethylene feedstock transition. The total environmental loads in 2018 were used as the baseline, to which we developed the scenarios of the Chinese ethylene industry in 2030 and 2050. Based on the weighting method (Qian et al., 2022), we evaluated the total environmental loadings of China's ethylene sectors in 2030 and 2050.

In the base year 2018, China's ethylene production was 18.41 Mt., with contributions from the four routes of ethane-fed ETE (184 Kt, 10‰), naphtha-fed OTE (15.28 Mt.; 83%), coal-fed CMTE (2.76 Mt.; 15%), and the bio-based BETE (184 Kt; 10‰). China's ethylene production capacity by 2030 and 2050 target is projected to reach 42.7 Mt. and 55 Mt., respectively (CPCIF, 2019a; Chen et al., 2018; Fig. S1). To peak emissions, the Chinese government calls for eliminating inefficient coal-fed ethylene plants with an annual capacity below 300 by 2025 (The People's Republic of China, 2022). Therefore, referring to the baseline, we developed 2030 and 2050 scenarios to evaluate the environmental burdens of the ethylene industry. The specific scenarios are as follows.

Scenario A: Coal-based CMTE production capacity rapidly grows, and the naphtha-based OTE route gradually decreases. **Scenario B:** CMTE production capacity gradually decreases, contrasting the rapid growth in the ETE capacity that uses ethane as feedstock; maintaining a slight increase in CMTE production. **Scenario C:** Extreme sustainability scenario, where the ethane-fed route expands with the percentage of the coal-based route remaining unchanged as the 2020 baseline. Table S1 details the predefined scenarios. During scenario analysis, the environmental impacts per tonne of ethylene product (i.e., 12 midpoint indicators and ECER index) were generated by the eFootprint system. These outputs were then used as inputs for scenario analysis to quantify the total environmental loads of China's ethylene industry.

3. Results and discussion

3.1. Midpoint life-cycle assessment

Fig. 2 shows the 12 midpoint environmental impacts of the four production routes. For climate burden, the CMTE route has the highest GWP metric averaging 12.1 $tCO_2e\ t^{-1}$, much higher than the ETE route (3.9 $tCO_2e\ t^{-1}$), OTE route (2.7 $tCO_2e\ t^{-1}$) and BETE route (4.3 $tCO_2e\ t^{-1}$). The ethane-fed ETE route performs better regarding PED, WU, AP, and RI impacts, which is only 20–44% of the CMTE route. The coal-based CMTE route generates the most severe GWP, PED, WU, and RI loads, while the bio-based BETE route is 1–3 times lower than those for the CMTE route. The BETE route has the highest stress for the AP, EP, ODP, POFP, IRP, ET, and HT-cancer metrics, which are 2–8 times higher than the ETE route. The lowest environmental burdens were observed in the conventional OTE route for all 12 metrics.

Notably, although carbon emissions of the emerging ETE route are 64% lower than those of the CMTE route, its ADP impact is 3–4 times higher than other routes. This trade-off is present among the 12 midpoint indicators of the four routes. Therefore, directly comparing the environmental performance of the four ethylene routes is difficult using the midpoint method. For example, replacing the CMTE route with the ETE route reduces carbon emissions, primary energy, and water consumption but increases the ADP load by three. Ethylene production includes two processes, i.e., raw materials extraction and ethylene production. Environmental burdens are sourced from different processes. For the ETE route, the upstream ethane production is responsible for 52–86% of the GWP, PED, WU, AP, ADP, RI, POFP, IRP, and HT-cancer impacts. For the coal-based CMTE route, the process of coal to methanol contributes 52–90% to all the 12 midpoint impacts, while the ethylene production process is only responsible for 10–48% of environmental burdens. The ethanol production process from corn on the BETE route contributes 68–99% to the environmental impact. In comparison, dehydrating ethanol to ethylene has <32% environmental impact.

To compare with prior evaluations, we searched the Web of Science database for the latest studies in the last decade. The keywords for the search were "TI=(ethylene OR olefin) and TI=(life cycle assessment or life-cycle* or LCA)". Conference papers were excluded from the analysis due to the lack of peer review and the difficulty of ensuring quality. We selected 21 articles for further review. Then, we selectively compared the commonly used metrics (e.g., GWP, PED, and WU) with our estimates (Fig. 3 and Table S3).

Our mean climate burden GWP of the ETE route (3.9 $tCO_2e\ t^{-1}$) slightly exceeds the estimates of Yao et al. (2016; 3.1 $tCO_2e\ t^{-1}$) and Zhao et al. (2014; 2.2 $tCO_2e\ t^{-1}$) at the statistical significance level of p-value<0.01. This deficiency lies in Yao et al. (2016) are based on more environmentally friendly steam turbines and compressors to process ethane feedstock. Zhao et al. (2014) only focus on the single GHG of CO_2, contrasting ours, including CO_2, CH_4, NO_x, etc., built-in the balance LCA modeling system. The GHG emissions of the OTE route are higher than the two reports of Yang and You, (2017; 1.2 $tCO_2e\ t^{-1}$) and Zhao et al. (2014; 1.4 $tCO_2e\ t^{-1}$). This is because the former models ethylene production by upgraded ethane-steam cracking and propane dehydrogenation technologies, while the latter is based on a high

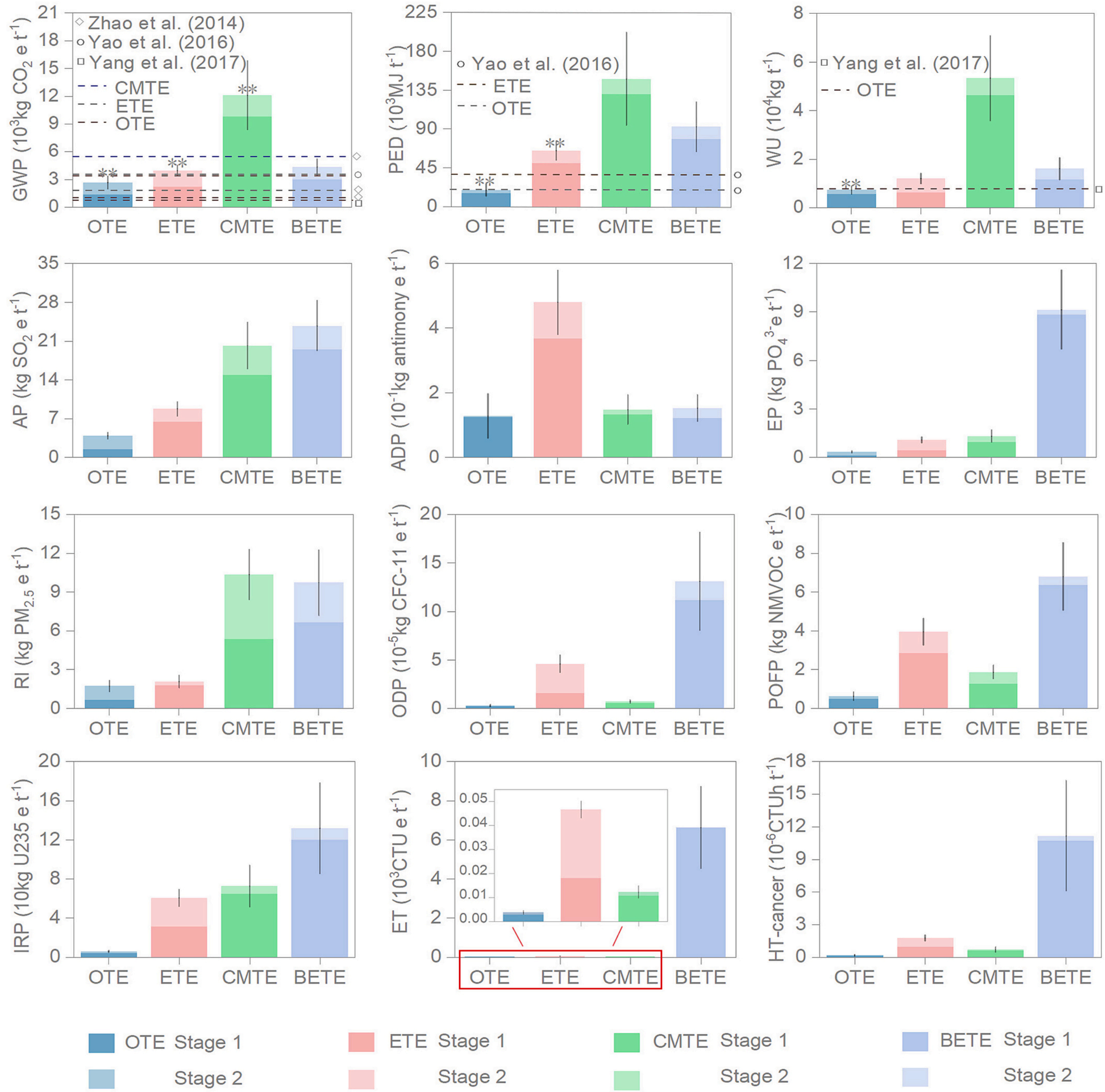

Fig. 2. Life-cycle midpoint assessment for the four ethylene production routes. Uncertainties were introduced from foreground and background data. The whiskers represent the 5th and 95th percentiles. ** represents the statistically significant levels of p-value<0.01. Stage 1 of OTE route refers to naphtha production and stage 2 to steam cracking to ethylene, stage 1 of the ETE route refers to ethane production and stage 2 refers to ethane to ethylene, stage 1 of the CMTE route refers to coal to methanol and stage 2 refers to methanol to olefins, the route's stage 1 of BETE route refers to corn to ethanol and stage 2 refers to ethanol dehydration to ethylene.

number of by-products, with an ethylene fraction coefficient (0.33) much lower than ours of 0.76. For the OTE route, the climate burdens of Yao et al. (2016) (3.1 $tCO_{2}e\ t^{-1}$) are higher than that of this study.

For energy consumption, the environmental impact of the ETE route in this paper is 65.4 GJ t^{-1}. The efficient technology application improves energy efficiency, making Yao et al. (2016; 26.2 GJ t^{-1}) substantially lower their energy metric than our estimate. The energy demand of the OTE route from Yao et al. (2016; 42.3 GJ t^{-1}) was considerably higher than ours (19.4 GJ t^{-1}). Notably, the coal-based CMTE route consumed the most volume of water resources (WU; 53.4 $m^3\ t^{-1}$), followed by the BETE (16.1 $m^3\ t^{-1}$), ETE (12 $m^3\ t^{-1}$), and OTE route (7.2 $m^3\ t^{-1}$) that is lower than the estimate of Yang and You, (2017; 11.3 $m^3\ t^{-1}$).

Except Yao et al. (2016), Yang and You (2017), and Zhao et al. (2014), we failed to directly compare our estimate with others because of inconsistent functional units and system boundaries (Table S3). However, we still describe the general features. For an example of bio-based ethylene, most current feedstock outside China depends on maize (Ghanta et al., 2014; Alonso-Farinas et al., 2018) and poplar (Liptow et al., 2013), whereas China's is on crops such as maize (Hong et al., 2014), cassava (Yang et al., 2018) and straw (Zhao et al., 2018). Chinese ethylene or olefin research typically focuses on cheap coal as feedstock (Xiang et al., 2014a, 2014b, 2015a, 2015b, 2016a, 2016b; Gao et al., 2018), while the US context study focuses on light alkane as by-

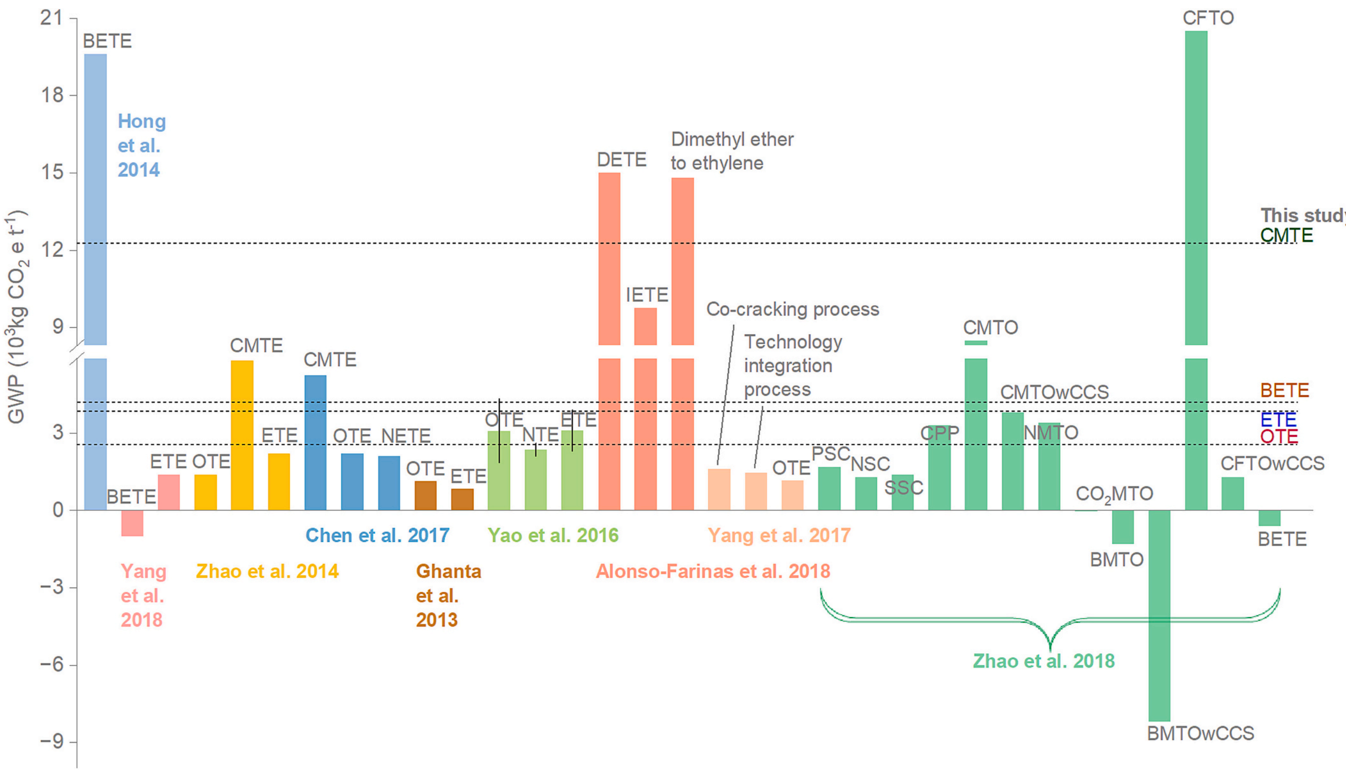

Fig. 3. Summary of reviewed climate burdens of varied ethylene production routes. Route abbreviations include bioethanol to ethylene (BETE), ethane to ethylene (ETE), naphtha to ethylene (OTE), coal-based methanol to ethylene (CMTE), natural gas-based methanol to ethylene (NMTE), natural gas to ethylene (NTE), direct/indirect dehydration of ethanol to ethylene (DETE/IETE), petroleum steam cracking (PSC), natural gas liquid/steam cracking to ethylene (NSC/SSC), heavy oil catalytic cracking process(CPP), coal to methanol to ethylene(CMTO), natural gas to methanol to ethylene(NMTO), carbon dioxide to methanol to ethylene (CO_2MTO), biological (maize, sugar cane) to methanol to ethylene (BMTO), coal-based syngas and olefin separation (CFTO and CFTOwCCS). Table S3 gives the detail.

products from shale gas explorations (He and You, 2016). German background study, e.g., Keller et al. (2020), compares the environmental sustainability of multiple feedstocks of crude oil, shale gas, wood, corn, solid waste, and flue gas.

Prior studies differ in allocating the environmental burdens between ethylene products and by-products. For example, Yang et al. (2018) applied the economic method; Yang and You (2017), He and You (2016) and Ren et al. (2008) combined the mass and economical method; Alonso-Farinas et al. (2018) used the energy and economical way; Ghanta et al. (2014) applied calorific value method. Hong et al. (2014), Zhao et al. (2014), Chen et al. (2017, 2018), Yao et al. (2016), Gao et al. (2018), and Keller et al. (2020), like this study, are based on mass allocation approaches.

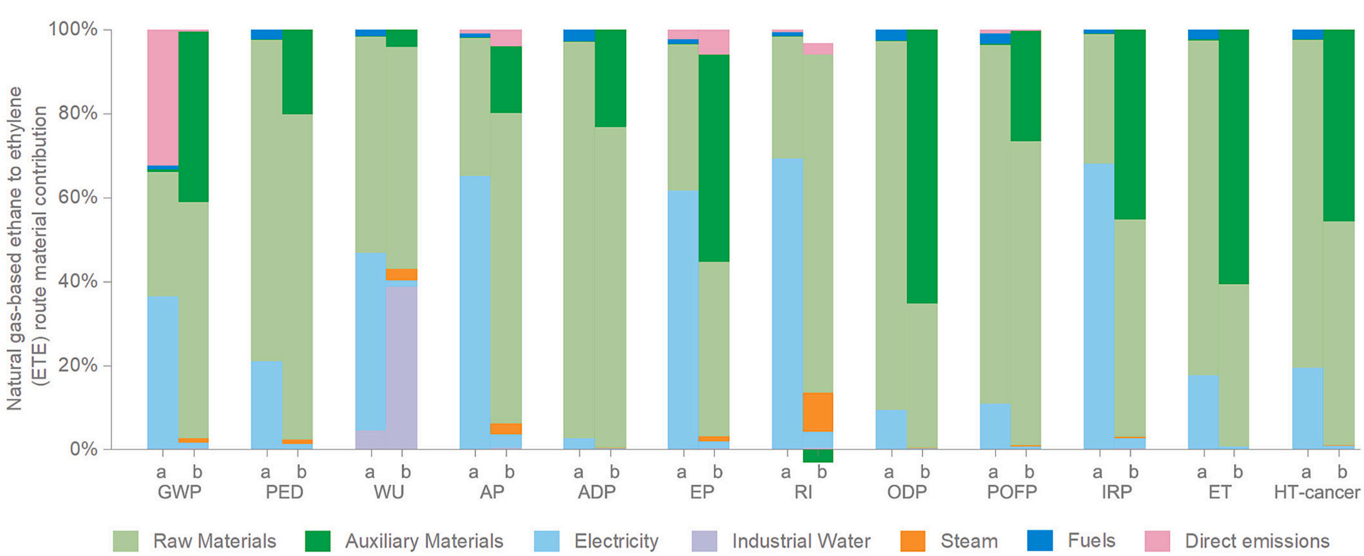

Fig. 4. Material contribution to environmental impacts at 12 midpoints for the four ethylene production routes. **(a)** represents the material contribution of the ethylene production stage for each route. **(b)** represents the material contribution at the upstream feedstock production stage.

3.2. Materials contribution to environmental impact

Material contributions to the 12 categories of environmental impacts vary across production routes. Fig. 4 exemplifies the contribution to the ETE route. The raw material of ethane is responsible for the largest contribution (52–86%) to the nine categories of environmental burdens, including GWP, PED, WU, AP, ADP, RI, POFP, IRP, and HT-cancer. Besides ethane, hydrogen dominates 88% of the environmental impacts associated with all auxiliary materials. Notably, the ETE route includes the steam recovery during the ethylene production process, which offsets the environmental burdens of all 12 categories by 25–45%.

For the coal-based CMTE route, methanol as raw material dominates the environmental impacts of ADP load (89%) and RI load (52%); and is responsible for 81% of GWP burdens or 8% higher than the direct GHGs emissions. Similarly, 90–99% of EP, POFP, IRP, ET, and HT-cancer environmental loads of the emerging BETE route are derived from ethanol consumption. For the naphtha-fed OTE route, raw materials contribute the most to ADP (97%) and ODP (88%) burdens, contrasting its 40% GWP, 31% AP, and 45% EP loads directly sourced from the ethylene factory. Figs. S2-S4 detail the materials contributions of the ETE, OTE, and CMTE routes.

3.3. Comprehensive evaluation on China's ECER index

Fig. 5 shows the comprehensive ECER metric of the four routes. The emerging ETE route that uses ethane as feedstock underperforms the conventional naphtha-fed OTE route in environmental friendliness. However, the ETE route is better than its coal-fed CMTE and bio-based BETE peers, lowering the ECER values by 62% and 33%, respectively. Carbon dioxide emissions account for 44% ECER index of the ETE ethylene production route, higher than the share of 20–33% for the other three ethylene production routes. By contrast, primary energy consumption (PED) accounts for 47%, 45%, and 41% of the ECER metrics of the ETE, CMTE, and BETE routes, respectively.

The raw materials contribute dominantly to the ECER, like to the 12 midpoints, for all four production routes. Besides, auxiliary materials, such as hydrogen, propane, and methane, are responsible for 25% of ECER impacts of the ETT route, among which hydrogen consumption shares 19% of the total loads from all auxiliary materials. Steam use takes up 11–14% of the environmental impacts of the OTE, CMTE, and BETE routes. Table S4 gives the detail.

3.4. Sensitivity analysis

Sensitivity analysis demonstrates that the RI impact is most sensitive to changes in the continuity and stability of ethane inputs. For example, a 10% increase in ethane use raises the RI load of ETE by 8%, along with a 6% increase in the ECER index. Therefore, reducing the upstream environmental burdens of ethane extraction and separation from shale gas is essential to improve the environmental performance of the ETE route. Contrastingly, increasing hydrogen input slightly reduces the RI impact. For example, a 10% increase in hydrogen use lowers the targeted RI metrics by 1.2%. The likely reason is that hydrogen is used as a fuel in the ethylene cracker, reducing PM2.5 emissions. For the CMTE route, the methanol input was observed with the most significant impact on the variations of ADP load. For example, a 5% reduction in methanol input decreased an 8% decline in the ADP burdens and an equivalent rise in the ECER metrics. The sensitivity analysis results for the four ethylene routes are shown in Figs. S5-S8.

3.5. Overall burdens of ethylene industry

China's ethylene production is expected to reach 42.7 Mt. and 55 Mt. by 2030 and 2050, respectively (CPCIF, 2019a; Chen et al., 2018). Based on the results of the life-cycle environmental impacts of per tonne ethylene (Section 3.1) and the predefined ethylene industry scenarios (Table S1), we quantified the varied overall environmental loads of China's ethylene industry in 2030 and 2050 (Fig. 6).

In the 2018 baseline, total GHG emissions, i.e., the mean (sd; [quantiles 5th and 95th]), from China's ethylene sector were 76(15; [51,101]) MtCO_2e. The mean amount is equal to 84% of social China's ethylene industry as an economy in the same year (CEADs, 2020). Regarding China's ethylene industry as an economy, we estimated its emissions are comparable to Romania's total society-wide GHG emissions (75 MtCO_2e) or Colombia's (79 MtCO_2e; Climate Watch, 2018). The water consumption of China's ethylene sector reached 262(57; [168, 352]) Mt., i.e., equivalent to 4–9% of Beijing's residential and domestic water consumption or 11–22% of China's total industrial water consumption (MWRC, 2019).

Referring to the 2018 baseline, China's ethylene sector growth under the three scenarios leads to a 145–472 (224–1207%) increase in the total loads of all the 12 environmental impact midpoints by 2030(2050). If the coal-based CMTE route continued to expand in equal proportions as the 2018 base year (Scenario A), the total GHG emissions and water consumption would increase by 258(453)% and 307(552)%, respectively, in 2030(2050). When the ethane-fed ETE route replaced 8(26)% production of the coal-fed CMTE route, the environmental loads would decrease by 15–23(12–24)% for GWP, PED, WU, AP, and RI, but increase other impacts by 12–91(10–124)%. If the ETE route continued to rise to 40% production capacity, and the share of the coal-fed CMTE route remained constant (Scenario C), the total GWP, PED, WU, AP, and RI loads would be 17–27(15–30)% lower than the baseline, while the

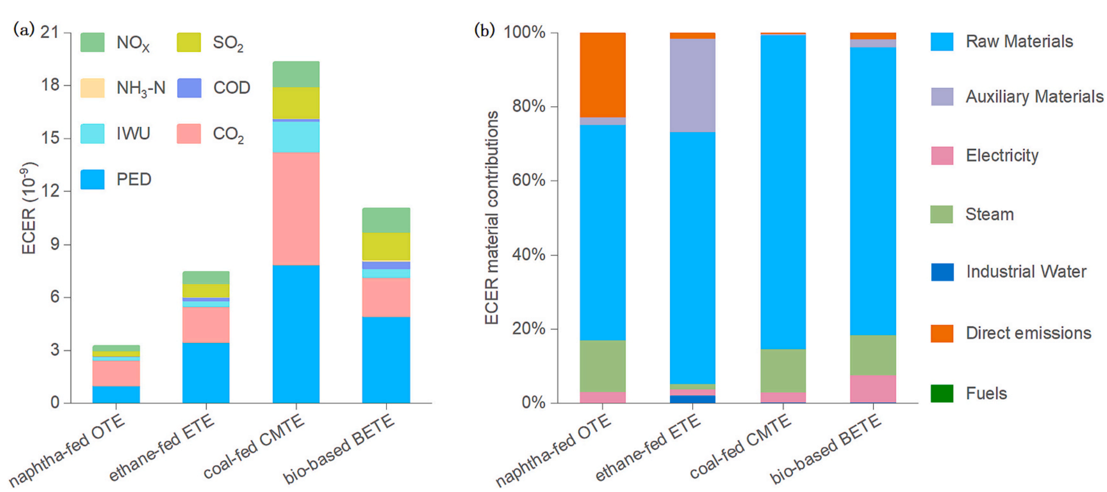

Fig. 5. Comprehensive comparison of (a) ECER index and (b) the material contribution to the ECER index of the four ethylene routes.

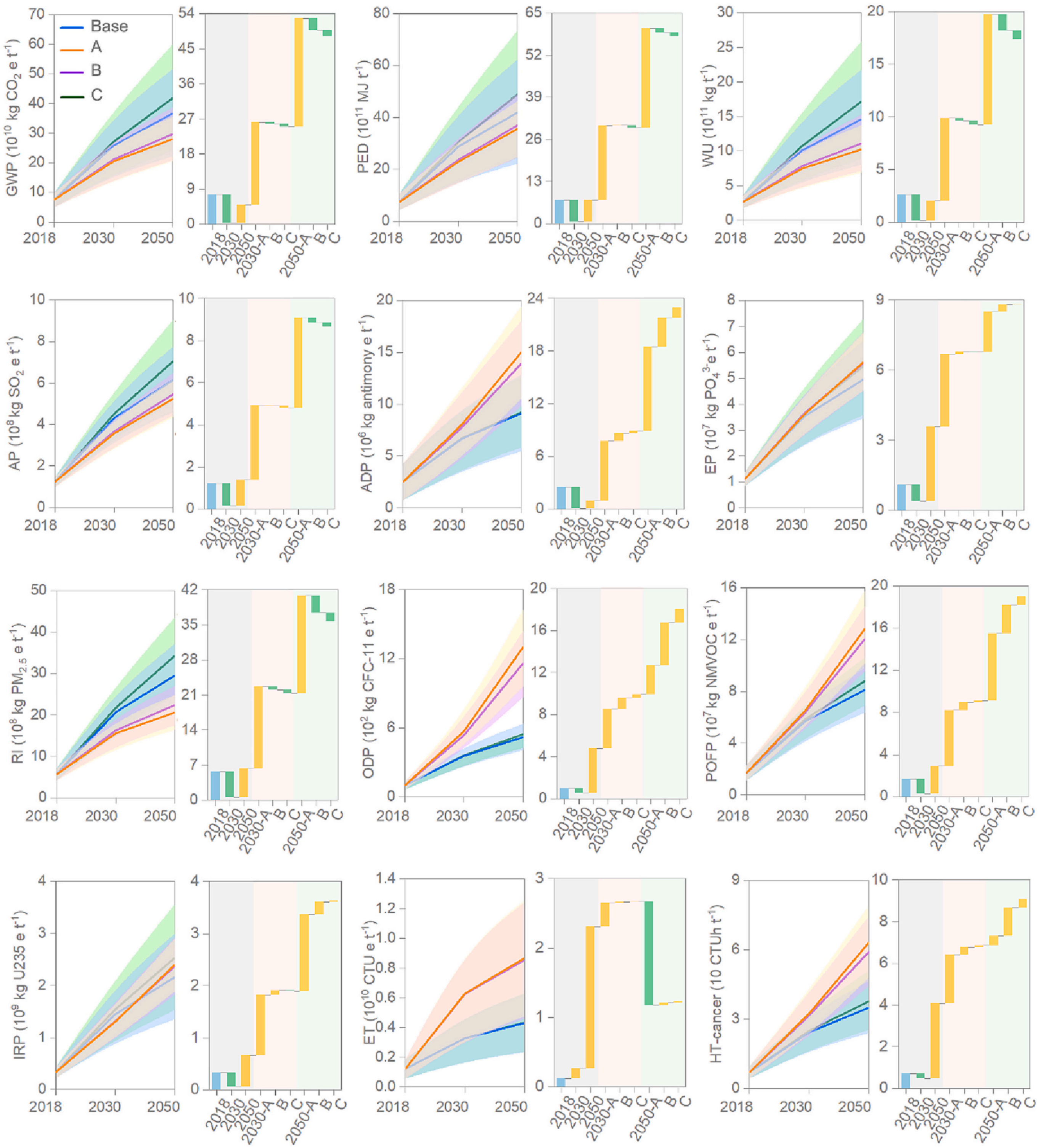

Fig. 6. The overall environmental burdens of China's ethylene industry in 2030 and 2050 under feedstock scenarios referring to the 2018 baseline. Scenarios a, b, and c reflect three levels of fast, slow, and constant growth in coal feedstock consumption. Uncertainties are sourced from the LCA models, quantified by Monte Carlo simulations. Background color: The grey represents the base scenario in 2018, 2030, and 2050, the red represents the three scenarios A, B, and C for 2030, and the green represents the three scenarios for 2050. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

remaining impacts increase by 15–92(11–149)% in 2030(2050). Notably, using ethane to replace coal in ethylene production would reduce the environmental load per tonne of ethylene product by 2–25% in 2030 and by 6–42% in 2050. However, due to continued industrial expansion, the total environmental burden on the Chinese ethylene industry will still increase by 1–44% in 2030 and 6–68% in 2050.

4. Conclusion

The shale gas revolution is transitioning China's feedstock of ethylene production. This transition alters the environmental burdens of China's ethylene industry because the environmental performance varies across production routes. We compared the life-cycle environmental performance of four ethylene routes and the overall impacts under varied ethylene industry scenarios.

Trade-offs across the 12 midpoint indicators impede directly comparing the environmental sustainability of the four ethylene routes. The ethane-based ETE route performs better in terms of GWP, PED and WU indicators, only 22–44% of the CMTE route. China's contextual ECER index overcomes the trade-off issue, suggesting that the ethane-fed ETE route and naphtha-fed OTE route outperform the coal-fed CMTE route in environmental friendliness (62% and 83% lower than coal-based routes). Raw material consumption is the key to determining the environmental performance of the four ethylene routes. Steam recovery offsets >40% of the environmental loads of the ETE route. Therefore, replacing the coal-based CMTE route with the ETE route contributes to less environmental pressure on China's ethylene industry. Considering China as the global second largest ethylene producer with soaring capacity, our estimates provide a reference for promoting the sustainability of the chemical manufacturing industry that uses ethylene as a primary material.

CRediT authorship contribution statement

Huimin Qian: Data curation, Investigation, Software, Visualization, Writing – original draft. **Yueru Zhao:** Data curation, Formal analysis, Investigation, Writing – original draft. **Fen Qin:** Formal analysis, Visualization. **Guobao Song:** Conceptualization, Methodology, Validation, Supervision, Writing – review & editing.

Declaration of Competing Interest

All authors (including Huimin Qian, Yueru Zhao, Fen Qin, Guobao Song) have no conflicts of interest to declare.

Data availability

All data used in the submission have been include in the Supplementary Information.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.eiar.2023.107152.

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