Supplementary Information for

Net-zero transition of the global chemical industry with CO_2-feedstock by 2050: feasible yet challenging

Jing Huo,*[a,b] Zhanyun Wang,[a,b,c] Christopher Oberschelp,[a,b] Gonzalo Guillén-Gosálbez[b,d] and Stefanie Hellweg[a,b]

Author Information:

[a] Chair of Ecological Systems Design, Institute of Environmental Engineering, ETH Zürich, John-von-Neumann-Weg 9, 8093, Zürich, Switzerland. E-mail: jhuo@ethz.ch

[b] National Centre of Competence in Research (NCCR) Catalysis, ETH Zürich, Zürich, Switzerland

[c] Empa-Swiss Federal Laboratories for Materials Science and Technology, Technology and Society Laboratory, Lerchenfeldstrasse 5, CH-9014 St. Gallen, Switzerland

[d] Sustainable Process Systems Engineering Lab, Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog-Weg 1, 8093, Zürich, Switzerland

Correspondence and requests for materials should be addressed to Jing Huo: jhuo@ethz.ch

Table of Contents

S0 Definitions and abbreviations

S0.1 Countries and regions

Table S1 Region abbreviations

Region abbreviation	Region
CN	China
EU	European Union (EU28, see Table S2)
IN	India
JP	Japan
KR	Republic of Korea
RAF	Region Africa
RME	Region Middle East
RU	Russian Federations
US	United States of America
RoW	Rest of the World
GLO	Global

Table S2 Region definitions

Region name	Included countries
European Union (EU)	Austria, Belgium, Bulgaria, Croatia, Cyprus, Czechia, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, United Kingdom of Great Britain and Northern Ireland
Region Africa (RAF)	Algeria, Angola, Benin, Botswana, Burkina Faso, Burundi, Cabo Verde, Cameroon, Central African Republic, Chad, Comoros, Congo, Côte d'Ivoire, Democratic Republic of the Congo, Djibouti, Egypt, Equatorial Guinea, Eritrea, Eswatini, Ethiopia, Gabon, Gambia (Republic of the), Ghana, Guinea, Guinea Bissau, Kenya, Lesotho, Liberia, Libya, Madagascar, Malawi, Mali, Mauritania, Mauritius, Morocco, Mozambique, Namibia, Niger, Nigeria, Rwanda, Sao Tome and Principe, Senegal, Seychelles, Sierra Leone, Somalia, South Africa, South Sudan, Sudan, Togo, Tunisia, Uganda, United Republic of Tanzania, Zambia, Zimbabwe
Region Middle East (RME)	Bahrain, Iran (Islamic Republic of), Iraq, Jordan, Kuwait, Lebanon, Oman, Qatar, Saudi Arabia, Syrian Arab Republic, United Arab Emirates, Yemen

S0.2 Organizations and projects

Table S3 Organization and project abbreviations

Abbreviation	Organizations/Projects
FAO	Food and Agriculture Organization of the United Nations
IEA	The International Energy Agency
IEAGHG	The International Energy Agency Greenhouse Gas R&D Programme
IPCC	The Intergovernmental Panel on Climate Change
JRC	Joint Research Center of the European Union
USGS	U.S. Geological Survey

S0.3 Scenarios defined by IEA

In this study, we refer to the following scenarios (Table S4) defined by IEA in their various reports.

Table S4 IEA scenarios abbreviations

Scenario abbreviation	Scenario	Appeared in
2DS	2 Degree Scenario	*Cement Technology Roadmap*[1]
STEPs	Stated Policies Scenario	*Iron and Steel Technology Roadmap*[2] *World Energy Outlook 2020*[3] *World Energy Outlook 2021*[4]
SDS	Sustainable Development Scenario	*Iron and Steel Technology Roadmap*[2] *World Energy Outlook 2020*[3] *World Energy Outlook 2021*[4]
NZE	Net Zero Emissions by 2050 Scenario	*Net Zero Emission Roadmap 2050*[5] *World Energy Outlook 2021*[4]

S0.4 Units

Table S5 Unit abbreviations

Unit abbreviation	Unit
kg	kilogram
Mt	Megatonne
Gt	Gigatonne
km	kilometer
MJ	Megajoule
TJ	Terajoule
kWh	kilowatt-hour
GWh	Gigawatt-hour
TWh	Terawatt-hour
MW	Megawatt
GW	Gigawatt
DALY	Disability-Adjusted Life Years

S0.5 Other abbreviations

Table S6 Other abbreviations appeared in this study

Abbreviation	Meaning
BAT	Best-Available Technology
BF-BOF	Blast Furnace-Basic Oxygen Furnace (steel production route)
BTX	Benzene, Toluene, Xylene
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilization

CCUS	Carbon Capture, Utilization and Storage
CHP	Combined Heat and Power
CO_2	Carbon Dioxide
DRI-EAF	Direct Reducing Iron-Electric Arc Furnace (steel production route)
EMO	Environmental Merit Order
GDP	Gross Domestic Product
GFPMX	Global Forest Products Model
GHG	Greenhouse gas
GWP	Global Warming Potential
HVC	High Value Chemicals, including ethylene, propylene, benzene, toluene, and xylenes
LCA	Life Cycle Assessment
MEA	Monoethanolamine
MTA	Methanol-To-Aromatics
MTO	Methanol-To-Olefins
NH3	Ammonia
NO_X	Nitrogen oxides
PM	Particulate matter
SO_2	Sulfur dioxide
SR-BOF	Smelting Reduction-Basic Oxygen Furnace (steel production route)
TRL	Technology Readiness Level

S1 Supporting details on methods

S1.1 CO_2 supply from power and industrial sectors

CO_2 were assumed to be supplied from power, steel, cement, and pulp sectors in 2050. Table S7 summarizes the key parameters affecting CO_2 emissions from each sector and lists the corresponding tables and paragraphs within this ESI for more detailed descriptions.

Table S7 Parameters affecting CO_2 emissions, by sector

Sectors	Suppliers	Parameters	Location in this ESI
Power	Coal-, natural gas-, solid biomass-fired power plants	Power generation amount	Table S15, Section S1.1.1.1
		Net electrical efficiency	Table S12, Table S13
		CO_2 emission factors of fuel combustion	Table S14
Steel	Integrated steel mills with BF-BOF, DRI-EAF, SR-BOF routes	Steel production volume	Table S22, Section S1.1.2.1
		Specific CO_2 emission factors of each production route	Table S18, Table S19, Section 0
Cement	Cement kilns	Cement production volume	Table S28, Section S1.1.3.1
		Clinker factor	Table S25, Section S1.1.3.2
		Thermal energy consumption	Table S26, Section S1.1.3.2
		Fuel mix	Table S27
		CO_2 emission factors of fuel combustion	Table S14
Pulp	Kraft pulp mills	Kraft pulp production volume	Table S30, Section S1.1.4.1
		Specific biogenic CO_2 emission factors	Section S1.1.4.2
		Thermal energy consumption of lime kilns	Section S1.1.4.2
		Fuel mix of lime kilns	Table S27
		CO_2 emission factors of fuel combustion	Table S14

S1.1.1 CO_2 emission scenarios from power plants

S1.1.1.1 Projection of electricity generation amount

IEA's *World Energy Outlook 2021*[4] projected global and regional electricity generation by fuel type in 2050 under different scenarios. In this study, IEA's projections under the Stated Policies Scenario (STEPs) were used for the high-emission scenario, and the low-emission scenario was set to align with IEA's Net Zero Emissions by 2050 Scenario (NZE).

However, only global projections are freely available for NZE, while for regional electricity generation, Sustainable Development Scenario (SDS) represents the most ambitious scenario with data that are freely available. Therefore, regional electricity generation with each fuel type (except biomass-fired and hydro electricity generation) under NZE was obtained by multiplying those under SDS with an extrapolating ratio as calculated in Table S8.

Table S8 Extrapolating ratio converting regional electricity generation under SDS to regional electricity generation under NZE

Type	A: Global generation in 2050 (NZE) (TWh)	B: Global generation in 2050 (SDS) (TWh)	Extrapolating ratio (A/B)
Total	71164	57950	1.23
Coal	663	1088	0.61

Oil	6	119	0.05
Natural gas	922	2755	0.33
Nuclear	5497	4714	1.17
Wind	24785	17577	1.41
Solar PV	23469	17433	1.35

For biomass-fired and hydro electricity generation, only global projection data are freely available in IEA's *World Energy Outlook 2021*. However, regional projections till 2040 were reported in an earlier version, i.e., IEA's *World Energy Outlook 2020*[3] under the STEPs and SDS scenarios. In this study, these values in 2040 were multiplied by the corresponding extrapolating ratio (specified in Table S9) to estimate regional projections of biomass-fired and hydro electricity generation in 2050, under high- and low-emission scenarios.

Table S9 Extrapolating ratio converting regional biomass-fired and hydro electricity generation projections from 2040 to 2050

	High-emission scenario			Low-emission scenario		
	A: Global generation in 2050 (STEPs)[4] (TWh)	B: Global generation in 2040 (STEPs)[3] (TWh)	Extrapolating ratio (A/B)	A: Global generation in 2050 (NZE)[4] (TWh)	B: Global generation in 2040 (SDS)[3] (TWh)	Extrapolating ratio (A/B)
Biomass	1852	1410	1.31	4121	2155	1.91
Hydro	6739	5919	1.14	8461	6690	1.26

For the Republic of Korea, since no data from IEA are freely available, the Current Policy Scenario and Net Zero 2050 Scenario from a Korea-focused study[6] were used instead for the high- and low-emission scenarios, respectively.

Biomass used in power plants is further divided into solid and liquid biofuels, and biogases. Regional electricity generation from the three fuel types in "main activity producer electricity plants" and "main activity producer CHP plants" in 2019 was reported in the "*Extended World Energy Balances*" in IEA's *World Energy Statistics and Balances* (CHP stands for combined heat and power).[7] The relative shares of the three biomass types were assumed to be the same in 2050 in all regions. If the regions have no biomass-fueled main activity producer electricity plants or CHP plants in 2019 according to IEA (China and Russian Federation), the global average share was used instead (Table S10).

Table S10 Share of electricity generation from the three biomass types, by region

Region	Solid biofuels	Liquid biofuels	Biogases
CN	No data, use the global average		
EU	58%	4%	38%
IN	0%	0%	100%
JP	98%	0%	2%
KR	64%	30%	6%
RAF	95%	0%	5%
RME	0%	0%	100%
RU	No data, use the global average		
US	56%	0%	44%

RoW	57%	14%	28%
GLO	61%	5%	34%

S1.1.1.2 *Specific carbon intensity*

Three types of power plants were considered in this study as potential CO_2 suppliers: coal-, natural gas-, and solid biomass-fueled power plants.

- Oil-fueled electricity generation (including liquid biofuel) represents 3.0% of global electricity generation in 2019, and this value is projected to decrease to 1.0% and 0.3% under high- and low-emission scenarios, respectively.[4] Therefore, fossil oil and liquid biofuel power plants were excluded from this study.
- Biogas-fueled power plants were also excluded because the maximum unit size of a biogas-fired gas turbine is only 15 Megawatt (MW).[8] The maximum annual CO_2 emissions from one unit is less than 0.06 Mt, assuming it runs at full capacity with current global average efficiency, which is smaller than 0.1 Mt CO_2/year emissions – the cut-off value of large point source emitters where carbon capture projects become economically appealing.[9]

Specific carbon intensity of electricity generation in one region/country depends on the net electrical efficiency there and the carbon intensity of corresponding fuels. The latest regional net electrical efficiencies were derived from the "*Extended World Energy Balances*" in IEA's *World Energy Statistics and Balances* for the year 2019.[7] The first step is to group the fuel products into fuel types (Table S11). Then, the fuel efficiency η per fuel type was calculated with the total regional fuel inputs ($\sum FI$, in TJ), electricity outputs ($\sum EO$, in GWh), and heat outputs ($\sum HO$, in TJ) in the case of combined heat and power (CHP) plants (Eqn(1)). Only "main activity producer electricity plants" and "main activity producer CHP plants" flows in the dataset were considered. The derived regional fuel-to-power efficiencies in 2019 are shown in Table S12.

$$\eta = \frac{3.6 \times \sum EO + \sum HO}{\sum FI} \tag{1}$$

Table S11 Products by fuel type (coal, natural gas, and solid biomass)

Fuel type	Products as in Extended World Energy Balances[7]
Coal	anthracite, coking coal, other bituminous coal, sub-bituminous coal, lignite, BKB, oil shale and oil sands, petroleum coke, coke oven coke, peat, peat products
Natural gas	natural gas
Solid biomass	primary solid biofuels

Table S12 Net electrical efficiency in 2019, by fuel type and region

Region	Fuel efficiency Coal non-CHP	Coal CHP	Natural gas non-CHP	Natural gas CHP	Solid biomass non-CHP	Solid biomass CHP
CN	39%	49%	56%	84%		

EU	38%	55%	53%	74%	38%	73%
IN	35%		41%			
JP	41%		52%		38%	
KR	39%		53%	70%	38%	75%
RAF	32%		40%		20%	
RME	37%		41%			
RU		55%		62%		
US	37%	49%	50%	73%	25%	79%
RoW	35%	62%	47%	51%	24%	23%
GLO	37%	50%	47%	65%	33%	70%

The efficiency will keep improving for main activity electricity / CHP producers. For the high-emission scenario, it was assumed that by 2050, the average electrical efficiency would improve by 15% from the level in 2019 in all regions (see main text for details), but not exceeding the best available technology (BAT) level identified by the Joint Research Center (JRC) of the European Union (Table S13).[8] For the low-emission scenario, all the combustion power plants in 2050 were set to operate with the efficiencies that corresponds to the BAT level. For CHPs, the BAT fuel efficiency depends on how much heat is generated. We assumed in 2050 the ratio of regional heat output to regional electricity output would remain the same as in 2019. The regional fuel efficiency for CHP plants was then calculated by interpolating the BAT fuel efficiency at 0% heat output (Table S13) and 90% at 100% heat output. For locations with no biomass-fired power plants in 2019, the projected global average efficiency for 2050 was used instead.

Table S13 BAT net electrical efficiency for main activity electricity producers, by fuel type

Fuel type	BAT net electrical efficiency	Scenario
Coal	46%	Coal-fired, ≥1000 MW_{th}, new unit
Gas	60.5%	CCGT, ≥600 MW_{th}, new unit
Solid biomass	38%	New unit

With electricity generation projections (P_{power}) by each fuel type (l) (TWh/year), the corresponding estimated fuel efficiency (η_l, %), and the default emission factors ($EF_{fuel,l}$, in tonne CO_2/TJ fuel) for each fuel product,[10] we then calculated the regional CO_2 emissions from each type of power plants ($E_{CO_2,power\ plants,i}$, Mt/year) under the two scenarios (Eqn (2)).

$$E_{CO_2,power\ plants,l} = \frac{3.6P_{power,l} \times EF_{fuel,l}}{1000\eta_l} \tag{2}$$

The default CO_2 emission factors by fuel type derived from the *IPCC Guidelines for National Greenhouse Gas Inventories*[10] were summarized in Table S14. It was assumed that these values stay the same across all scenarios. Specifically, since there are different products under the fuel type of coal with different emission factors, weighted regional average emission factors were calculated with the amount of each product input into the “main activity producer electricity plants” and “main activity producer CHP plants”.

Table S14 Default CO_2 emission factors, by fuel type and region

	Coal (tonne CO_2/TJ)	Natural gas (tonne CO_2/TJ)	Solid biomass (tonne CO_2/TJ)
CN	94.6	56.1	100
EU	98.2		
IN	95.1		
JP	94.7		
KR	94.8		
RAF	94.6		
RME	95.3		
RU	97.3		
US	95.9		
RoW	96.4		
GLO	95.3		

The regionalized projection of electricity generation by fuel type and the corresponding CO_2 emissions under the high- and low-emission scenarios are summarized in Table S15.

Table S15 Regionalized projection of electricity generation and the corresponding CO_2 emissions under high- and low-emission scenarios, by fuel type and region

Fuel	Region	High-emission scenario		Low-emission scenario	
		Electricity generation (TWh/year)	CO_2 emissions (Mt/year)	Electricity generation (TWh/year)	CO_2 emissions (Mt/year)
Coal	CN	3349	2874	449	358
	EU	15	13	12	10
	IN	947	805	67	50
	JP	65	48	31	23
	KR	0	0	0	0
	RAF	175	160	19	14
	RME	29	24	4	3
	RU	127	122	0	0
	US	55	45	31	23
	RoW	1530	1372	50	40
	GLO	6293	5463	663	520
Natural gas	CN	539	272	232	117
	EU	356	137	14	5
	IN	172	74	41	14
	JP	139	48	34	11
	KR	228	83	128	47
	RAF	705	307	69	23
	RME	1574	678	124	41
	RU	653	399	77	44
	US	1555	562	59	20
	RoW	2511	961	133	46
	GLO	8432	3520	909	368

Solid biomass	CN	311	362	630	734
	EU	188	235	357	447
	IN	0	0	0	0
	JP	91	86	135	128
	KR	24	23	45	42
	RAF	50	55	113	132
	RME	0	0	0	0
	RU	27	31	143	167
	US	78	110	252	296
	RoW	354	544	825	833
	GLO	1123	1447	2499	2779

S1.1.2 CO_2 emission scenarios from steel mills

S1.1.2.1 Projection of crude steel production volume

The regional production volumes of crude steel in 2019 by routes was summarized in the *Steel Statistical Yearbook 2020 concise version*.[11]

For the high-emission scenario in 2050, the annual growth rate of global and regional crude steel production projections was set according to the IEA's Stated Policy Scenario (STEPS) (see Table S16 for details).[2, 12]

Table S16 Crude steel production annual growth, from 2019 to 2050 under the high-emission scenario, by region

Region	Annual growth	Data source	Note
CN	-0.4%	2	
EU	0.2%	2	
IN	8.8%	2	
JP	-0.3%	12	projection for "Developed Asia and Oceania" as proxy
KR	-0.3%	12	projection for "Developed Asia and Oceania" as proxy
RAF	41.3%	12	
RME	3.7%	2	
RU	0.2%	2	the same growth rate as EU was assumed
US	0.8%	2	
GLO	1.3%	2	

The low-emission scenario was set to be 1.5°C pathways-compliant, under which more ambitious decarbonization measures are required in comparison to IEA's Sustainable Development Scenario (SDS), as researchers pointed out that the sector's greenhouse gas (GHG) budget till 2050 for keeping the temperature increase within 1.5°C will be exhausted by 2038 under SDS.[12] Therefore, for the low-emission scenario, the demand for crude steel was set to decrease by 10% relative to that in the SDS assuming a better material efficiency. The annual growth rates of crude steel production by region are shown in Table S17.

Table S17 Crude steel production annual growth, from 2019 to 2050 under the low-emission scenario, by region

Region	Annual growth	Data source	Note
CN	-1.1%		
EU	-0.8%		
IN	4.3%		
JP	-0.8%		the same growth rate as EU was assumed
KR	-0.8%	2	the same growth rate as EU was assumed
RAF	8.4%		
RME	1.7%		
RU	-0.8%		the same growth rate as EU was assumed
US	0.0%		
GLO	0.1%		

S1.1.2.2 Specific carbon intensity

CO_2 emissions from the steel sector come predominantly from three production routes, namely the blast furnace-basic oxygen furnace (BF-BOF) route, direct reduced iron-electric arc furnace (DRI-EAF) route, and the new smelting reduction-basic oxygen furnace (SR-BOF) route that was set to commercialize under the low-emission scenario in 2050.

For secondary steel making, CO_2 emissions come predominantly from power plants, which were addressed separately in Section S1.1.1. The regionalized baseline CO_2 intensities of the BF-BOF route in 2019 were summarized in Table S18. Due to data constraint, CO_2 intensities of the DRI-EAF and SR-BOF route reported by Material Economics (1.1 and 1.5 tonnes CO_2 per tonne steel, respectively)[13] were used in all regions as baseline.

Table S18 Specific CO_2 emission factors of the BF-BOF route, by region

Region	Specific CO_2 emission factors (tonne CO_2/tonne steel)	Data source	Note
CN	2.36	14	
EU	1.90	14	Weighted average of European countries included in the study (Spain, France, Germany, Italy, and Poland)
IN	2.79	14	
JP	1.92	14	
KR	2.34	14	
RAF	2.24	14	Global average was used as proxy
RME	2.24	14	Global average was used as proxy
RU	1.84	14	
US	1.83	14	
GLO	2.24	14	Weighted average of all countries included in the study (Canada, Spain, Mexico, United States, France, Russia, Japan, Germany, Italy, Brazil, Turkey, Republic of Korea, China, India, Poland)

Specific CO_2 emission factors of each production route was set to decrease by 15% under the high-emission scenario in 2050 as a result of energy efficiency improvement (see main text), as long as it is larger than the specific CO_2 emission factors with BAT (Table S19). Under the low-emission scenario, we assumed that the specific CO_2 emission factors of all three routes would match BAT.

Table S19 Specific CO_2 emission factors of BAT steel production, by route

Production route	Specific CO_2 emission factors (tonne CO_2/tonne steel)	Data source	Note
BF-BOF	1.60	[14]	
DRI-EAF (natural gas)	0.84	[15]	
SR-BOF	1.28		The emission factor of SR-BOF is 20% lower than BF-BOF.[14]

The share of each production route is another key factor affecting regional specific carbon intensities. For the high-emission scenario, we assumed that the share of regional production routes follows the stated policies scenario (STEPS) set by IEA.[2] For countries without detailed analysis, we assumed that Japan and Republic of Korea would follow similar production routes as EU, and Russia would follow that of the China.

Table S20 Share of different primary steel production routes under the high-emission scenario in 2050, by region, adapted from IEA[2]

Region	BF-BOF	SR-BOF	DRI-EAF (natural gas)	Other low-carbon routes	Secondary steelmaking	Note
CN	55%	0%	0%	0%	45%	
EU	44%	0%	2%	0%	54%	
IN	55%	0%	20%	0%	25%	
JP	44%	0%	2%	0%	54%	Same mix as EU was assumed
KR	44%	0%	2%	0%	54%	Same mix as EU was assumed
RAF	43%	0%	39%	0%	18%	
RME	3%	0%	72%	0%	25%	
RU	55%	0%	0%	0%	45%	Same mix as CN was assumed
US	28%	0%	35%	0%	37%	
GLO	53%	0%	11%	0%	36%	

The low-emission scenario was set to align with IEA's Net Zero Emissions (NZE) scenario.[5] In particular, the global average share of secondary steelmaking would increase to 46% (in comparison to 38% under SDS). The share of other low-carbon production routes (e.g., hydrogen-based DRI-EAF and iron ore-electrolysis-EAF) would reach 23% on the global average (in comparison to 8% under SDS). Since NZE only analyzed the global overview, the difference of global shares between NZE and SDS (15% for other low-carbon routes and 8% for secondary steelmaking) was added to the regional shares under SDS for the low-emission scenario in this study. As a result, the ratio of other pathways (BF-BOF, SR-BOF and DRI-EAF) would decrease accordingly. However, the relative ratio among the three routes was kept the same as in SDS.

Table S21 Share of different primary steel production routes under the low-emission scenario in 2050, by region, adapted from IEA[2]

Region	BF-BOF	SR-BOF	DRI-EAF (natural gas)	Other low-carbon routes	Secondary steelmaking	Note
CN	19%	4%	0%	23%	54%	
EU	8%	1%	0%	26%	65%	
IN	17%	12%	7%	30%	33%	
JP	8%	1%	0%	26%	65%	Same mix as EU was assumed
KR	8%	1%	0%	26%	65%	Same mix as EU was assumed
RAF	24%	0%	15%	33%	28%	
RME	0%	0%	33%	29%	37%	
RU	19%	4%	0%	23%	54%	Same mix as CN was assumed
US	7%	0%	28%	14%	51%	
GLO	19%	5%	7%	23%	46%	

With steel production projections (P_{steel}, Mt/year), the share of each production route (f_j, %, j denotes BF-BOF, SR-BOF, or DRI-EAF), and the specific CO_2 emission factors of the corresponding production route ($EF_{steel,j}$, in tonne CO_2/tonne steel), we then calculated the regional CO_2 emissions from each type of steel mills ($E_{CO_2,steel\,mills,j}$, Mt/year) under the two scenarios (Eqn (3)).

$$E_{CO_2,steel\,mills,j} = P_{steel} \times f_j \times EF_{steel,j} \tag{3}$$

The regionalized projection of steel production by route and the corresponding CO_2 emissions under the high- and low-emission scenarios are summarized in Table S22.

Table S22 Projection of steel production and the corresponding CO_2 emissions under high- and low-emission scenarios, by route and region

Route	Region	High-emission scenario		Low-emission scenario	
		Steel production (Mt/year)	CO_2 emissions (Mt/year)	Steel production (Mt/year)	CO_2 emissions (Mt/year)
BF-BOF	CN	488	978	122	195
	EU	73	119	9	15
	IN	229	543	45	72
	JP	39	64	6	9
	KR	28	56	4	7
	RAF	102	194	15	24
	RME	3	6	0	0
	RU	42	66	10	16
	US	31	48	6	9
	RoW	322	511	149	239
	GLO	1357	2584	367	587
SR-BOF	CN	0	0	28	36
	EU	0	0	1	1

	IN	0	0	32	41
	JP	0	0	1	1
	KR	0	0	0	1
	RAF	0	0	0	0
	RME	0	0	0	0
	RU	0	0	2	3
	US	0	0	0	0
	RoW	0	0	40	51
	GLO	0	0	104	133
DRI-EAF	CN	0	0	0	0
	EU	3	3	0	0
	IN	83	78	18	15
	JP	2	2	0	0
	KR	1	1	0	0
	RAF	92	86	9	8
	RME	68	64	23	19
	RU	0	0	0	0
	US	38	36	25	21
	RoW	38	35	52	44
	GLO	326	305	126	106

S1.1.3 CO_2 emission scenarios from cement kilns

S1.1.3.1 Projection of cement production volume

Cement production in 2019 was reported by U.S. Geological Survey (USGS)[16] for selected regions. This data source was supplemented by the statistics from regional cement associations for KR,[17] and EU and RAF.[18]

For the high-emission scenario, the regionalized annual growth rate of cement production was set according to the high-variety case in IEA's *Technology Roadmap* for cement (Table S23*).*[1]

Table S23 Cement production annual growth, from 2019 to 2050 under the high-emission scenario, by region

Region	Annual growth	Data source	Note
CN	-0.8%	1	
EU	0.3%		Projection for "Europe" was used as proxy
IN	5.1%		
JP	0.3%		The same growth rate as EU was assumed
KR	0.3%		The same growth rate as EU was assumed
RAF	7.9%		
RME	0.8%		
RU	1.2%		Projection for "Eurasia" was used as proxy
US	2.0%		Projection for "America" was used as proxy
GLO	0.8%		

Since the IEA's *Technology Roadmap* for cement only examined pathways to keep the temperature increase within 2°C, it is plausible that more efforts would be required in the 1.5°C pathways-compatible low-emission scenario. Therefore, we assumed that the cement production outside China would be 10% lower than the low-variety case set by IEA. Projections for China based on annual consumption per capita and cement stocks per capita revealed that cement production in China would decrease drastically to 800 Mt/year,[19, 20] which was used for the low-emission scenario in this study. The regionalized annual growth rate of cement production was summarized in Table S24.

Table S24 Cement production annual growth, from 2019 to 2050 under the low-emission scenario, by region

Region	Annual growth	Data source	Note
CN	-2.1%	19, 20	Calculated with the assumption that the annual cement production in 2050 would drop to 800 Mt
EU	-0.3%	1	Projection for "Europe" was used as proxy
IN	3.6%	1	
JP	-0.3%	1	The same growth rate as EU was assumed
KR	-0.3%	1	The same growth rate as EU was assumed
RAF	5.9%	1	
RME	0.1%	1	
RU	0.4%	1	Projection for "Eurasia" was used as proxy
US	1.0%	1	Projection for "America" was used as proxy
GLO	-0.4%	1	

S1.1.3.2 Specific carbon intensity

Process emission ($EF_{cement\ process}$): the default CO_2 emissions from limestone calcination is 0.52 tonnes CO_2/tonne clinker.[10] This was considered to be the same in all scenarios.

Clinker factor (CF): clinker factor (tonne clinker/tonne cement) is the weight percentage of clinker in cement. Clinker production is the most energy intensive step during cement production. Therefore, reducing clinker factor can contribute to the reduction of CO_2 emissions.[1] The clinker factor depends on the required mechanical properties of its end-use applications. IEA set the clinker factor of 0.57 to be a key milestone for its NZE,[5] which was used in this study for all regions under the low-emission scenario. The regional clinker factors under the high-emission scenario were set according to IEA's 2 degree scenario (2DS) in 2030 (Table S25).[1]

Table S25 Clinker factor under the high-emission scenario, by region

Region	Clinker factor	Data source	Note
CN	0.58	1	
EU	0.67	1	Projection for "Europe" was used as proxy
IN	0.67	1	
JP	0.72	1	Projection for "Other Asia Pacific" was used as proxy
KR	0.72	1	Projection for "Other Asia Pacific" was used as proxy

RAF	0.70	1	
RME	0.66	1	
RU	0.72	1	Projection for “Eurasia” was used as proxy
US	0.67	1	Projection for “America” was used as proxy
GLO	0.66	1	

Thermal energy consumption (E_{th}): regional thermal energy consumption (in MJ/tonne clinker) under the high-emission scenario were set according to IEA’s 2DS in 2030 (Table S26).[1] For the low-emission scenario, the thermal energy consumption was set at the BAT level (2900 MJ/tonne clinker)[21] for all regions.

Table S26 Thermal energy consumption under the high-emission scenario, by region

Region	Thermal energy consumption (MJ/tonne clinker)	Data source	Note
CN	3040	1	
EU	3434	1	Projection for “Europe” was used as proxy
IN	2975	1	
JP	3542	1	Projection for “Other Asia Pacific” was used as proxy
KR	3542	1	
RAF	3673	1	
RME	3372	1	
RU	4523	1	Projection for “Eurasia” was used as proxy
US	3625	1	Projection for “America” was used as proxy
GLO	3323	1	

Fuel mix (r): fossil fuels are the predominant fuels used in the cement industry today. Alternative fuels such as biomass and industrial waste are increasingly used to reduce the carbon footprint of the industry.

For the high-emission scenario in 2050, the fuel mix was set to resemble 2DS in 2030 in IEA’s *Technology Roadmap* for cement.[1] For the low-emission scenario, the share of alternative fuels (biomass and industrial waste) was set to 60% for the Annex I Parties under the Kyoto Protocol (EU, JP, KR, US) and 35% for the non-Annex I Parties (CN, IN, RAF, RME, RU).[22] The relative shares among each fuel type within fossil fuels (i.e., coal, oil, and natural gas) and alternative fuels (i.e., biomass and industrial waste) were assumed to be the same as under the high-emission scenario. Table S27 summarizes the regional fuel mix under high- and low-emission scenarios.

Table S27 Fuel mix in cement kilns, by scenario and region

Region	Coal	Oil	Natural gas	Biomass	Industrial waste	Note
High-emission scenario						
CN	87%	0%	2%	4%	6%	
EU	22%	24%	14%	13%	27%	Projection for “Europe” was used as proxy
IN	56%	31%	0%	6%	8%	

JP	67%	4%	4%	10%	15%	Projection for “Other Asia Pacific” was used as proxy
KR	67%	4%	4%	10%	15%	Projection for “Other Asia Pacific” was used as proxy
RAF	7%	31%	46%	6%	10%	
RME	11%	38%	34%	7%	11%	
RU	21%	0%	68%	4%	7%	Projection for “Eurasia” was used as proxy
US	24%	37%	14%	8%	18%	Projection for “America” was used as proxy
GLO	56%	14%	13%	6%	11%	
Low-emission scenario						
CN	63%	0%	2%	14%	21%	
EU	15%	16%	9%	19%	41%	
IN	42%	23%	0%	15%	20%	
JP	36%	2%	2%	24%	36%	
KR	36%	2%	2%	24%	36%	
RAF	5%	24%	36%	12%	23%	
RME	9%	30%	27%	14%	21%	
RU	15%	0%	50%	14%	21%	
US	13%	20%	7%	17%	43%	
GLO	42%	11%	10%	14%	23%	

Specific emission factor (EF_{cement}): the specific fossil and biogenic CO_2 emission factors for a region (in tonne CO_2/tonne cement) was calculated using Eqn (4) and (5). The default emission factor for each fuel type k ($EF_{fuel,k}$) (tonne CO_2/TJ fuel) from the *IPCC Guidelines for National Greenhouse Gas Inventories* was used in the calculation.[10]

$$EF_{cement,fossil} = CF \times (EF_{cement\,process} + E_{th} \times \sum_{k} \frac{EF_{fuel,k} \times r_k}{10^6}) \tag{4}$$

k denotes individual types of fossil fuels (coal, oil, natural gas, and industrial waste).

$$EF_{cement,biogenic} = CF \times E_{th} \times EF_{biomass} \times r_{biomass} \tag{5}$$

With cement production projections (P_{steel}, Mt/year), and the specific CO_2 emission factors (EF_{cement}, in tonne CO_2/tonne cement), we then calculated the regional CO_2 emissions from each type of steel mills ($E_{CO_2,steel\,mills,j}$, Mt/year) under the two scenarios (Eqn (6)).

$$E_{CO_2,cement} = P_{cement} \times EF_{cement} \tag{6}$$

The regionalized projection of cement and the corresponding CO_2 emissions under the high- and low-emission scenarios are summarized in Table S28.

Table S28 Projection of cement production and the corresponding CO_2 emissions, by scenario and region

	High-emission scenario			Low-emission scenario		
Region	Cement production (Mt/year)	Fossil CO_2 emissions (Mt/year)	Biogenic CO_2 emissions (Mt/year)	Cement production (Mt/year)	Fossil CO_2 emissions (Mt/year)	Biogenic CO_2 emissions (Mt/year)

CN	1713	796	13	800	357	19
EU	202	110	6	165	73	5
IN	882	459	10	723	316	18
JP	59	35	1	48	21	2
KR	56	34	1	46	20	2
RAF	710	386	10	582	244	12
RME	204	103	3	167	70	4
RU	76	45	1	62	26	1
US	143	79	3	117	53	3
RoW	1097	687	24	899	404	18
GLO	5141	2734	73	3610	1586	84

S1.1.4 CO_2 emission scenarios from kraft pulp mills

S1.1.4.1 Projection of kraft pulp production volume

The regional production volume of kraft pulp in 2019 was summarized based on the database of Food and Agriculture Organization of the United Nations (FAO).[23] The Global Forest Products Model (GFPMX) predicts the consumption and production of forest products in 180 countries till 2070 based on population, Gross Domestic Product (GDP), local price and international trade.[24] The prediction of wood pulp production from the GFPMX was used in this study to derive the annual growth rate of kraft pulp production from 2019 to 2050 for the high-emission scenario. Under the low-emission scenario, the regional production was set to be 15% lower than that under the high-emission scenario, as this is in line with the IEA's NZE scenario.[25]

Table S29 Kraft production annual growth, from 2019 to 2050, by scenario and region

Region	Kraft production annual growth	
	High-emission scenario	Low-emission scenario
CN	1.4%	0.7%
EU	1.2%	0.5%
IN	9.1%	7.3%
JP	0.3%	-0.2%
KR	2.1%	1.3%
RAF	-0.5%	-0.9%
RME	0.8%	0.2%
RU	1.5%	0.8%
US	0.3%	-0.2%
GLO	1.1%	0.5%

S1.1.4.2 Specific carbon intensity

The main CO_2 emission sources at a kraft pulp mill include the kraft recovery boiler, multi-fuel boiler, and lime kiln.[26] In the kraft recovery boiler, woody materials in black liquor is combusted to produce energy for recycling of the cooking chemical. In the multi-fuel boiler, wood residuals from the wood handling unit are the main fuels. Additional fossil fuel is only required in the lime kiln to recover lime, which is then used to recover white liquor. The biogenic CO_2 emission factors were assumed to be the same as a reference mill reported by IEA Greenhouse Gas R&D Programme (IEAGHG)[26] (2.6 tonne CO_2/tonne kraft pulp) in all regions in this study due to a lack of regional data.

Kraft pulp mills were considered as net energy exporters. Biogenic CO_2 emissions are hence only related to how much biofuel is available for combustion. In this study, we assumed that black liquor and wood residue would continue to be used for energy recovery. Potential material valorization of lignin recovered from black liquor was not discussed in this paper. Therefore, the biogenic CO_2 emission factors of kraft pulp mills were assumed to be the same in 2050 as today.

For lime kilns on site of kraft pulp mills, we assumed that the thermal energy efficiency would increase by 15% from the level in 2019 to 1220 MJ/tonne kraft pulp under the high-emission scenario in 2050, and would be improved to the practical minimum level (1055 MJ/tonne kraft pulp)[27] under the low-emission scenario. The fuel mix used in the lime kiln was set to be the same as in the cement industry in all scenarios.

The fossil and biogenic CO_2 emissions from kraft pulp mills in a certain region (in Mt/year) is therefore calculated with Eqn. (7)-(8):

$$E_{fossil\ CO_2,pulp} = P_{pulp} \times \left(E_{th,lime\ kiln} \times \sum_m \frac{EF_{fossil\ fuel,m} \times r_m}{10^6}\right) \quad (7)$$

$$E_{biogenic\ CO_2,pulp} = P_{pulp} \times \left(2.6 + E_{th,lime\ kiln} \times \frac{EF_{biofuel} \times r_{biofuel}}{10^6}\right) \quad (8)$$

Where P_{pulp} stands for the annual production volume of kraft pulp (Mt/year), $E_{th,lime\ kiln}$ is the unit thermal energy consumption in the lime kiln (MJ/tonne kraft pulp), r_m and $EF_{fossil\ fuel,m}$ are the share of fuel m in the lime kiln and its corresponding CO_2 emission factors (tonne CO_2/TJ fuel) as from the *IPCC Guidelines for National Greenhouse Gas Inventories.*[10] $r_{biofuel}$ and $EF_{biofuel}$ are the share and emission factor of solid biomass as fuel in the lime kiln.

The regionalized projection of kraft pulp and the corresponding CO_2 emissions under the high- and low-emission scenarios are summarized in Table S30.

Table S30 Projection of kraft pulp production and the corresponding CO_2 emissions, by scenario and region

Region	High-emission scenario			Low-emission scenario		
	Kraft pulp production (Mt/year)	Fossil CO_2 emissions (Mt/year)	Biogenic CO_2 emissions (Mt/year)	Kraft pulp production (Mt/year)	Fossil CO_2 emissions (Mt/year)	Biogenic CO_2 emissions (Mt/year)
CN	14	2	38	12	1	32
EU	35	4	92	30	3	78
IN	9	1	24	8	1	21
JP	9	1	22	7	1	19
KR	1	0	2	1	0	2
RAF	1	0	2	1	0	2

RME	0	0	0	0	0	0
RU	8	1	21	7	1	18
US	49	5	128	42	4	109
RoW	70	8	183	60	6	155
GLO	196	21	511	167	15	436

S1.2 CO$_2$-feedstock demand from the chemical industry

S1.2.1 Production volumes of seven primary chemicals in 2050

Historical regional production volumes of the seven key chemicals and the corresponding data sources were summarized or estimated in Table S31 for the year of 2019. Their projected annual growth rates in production under high- and low- emission scenarios were reported in Table S33 and Table S34, respectively with detailed data sources and explanations. Due to data constraint, benzene, toluene, and xylene (BTX) aromatics were grouped together for the projections of production volumes.

Table S31 Production volumes of chemicals in 2019, by chemical and region

Chemicals	Region	Production volume in 2019 (Mt)	Data source	Data source category	Note
Urea	CN	53	[28]	Regional industrial association	
	EU	9	[29]	International industrial association	
	IN	24	[30]	United Nations	
	JP	<1	[30]	United Nations	
	KR	0	[30]	United Nations	
	RAF	11	[29]	International industrial association	
	RME	23	[29]	International industrial association	
	RU	9	[30]	United Nations	
	US	10	[31]	Governmental organization	
	RoW	37		Own estimation	Difference of global and regional production volumes
	GLO	177	[29]	International industrial association	
Methanol*	CN	36	[32]	Market insight report	Extrapolated from 2018 production volume, assuming 4% annual growth rate[33]
	EU	3	[32]	Market insight report	Extrapolated from 2018 production volume (sum of “Central Europe” and “West Europe” as proxy), assuming 4% annual growth rate[33]
	IN	<1	[34]	Governmental organization	
	JP	0	[32]	Market insight report	Extrapolated from 2018 production volume, assuming 4% annual growth rate[33]

	KR	0	[32]	Market insight report	Extrapolated from 2018 production volume, assuming 4% annual growth rate[33]
	RAF	3	[32]	Market insight report	Extrapolated from 2018 production volume, assuming 4% annual growth rate[33]
	RME	15	[32]	Market insight report	Extrapolated from 2018 production volume, assuming 4% annual growth rate[33]
	RU	4	[32]	Market insight report	Extrapolated from 2018 production volume (FSU as proxy), assuming 4% annual growth rate[33]
	US	6	[35]	Market insight report	
	RoW	15		Own estimation	Difference of global and regional production volumes
	GLO	82	[32]	Market insight report	Extrapolated from 2018 production volume, assuming 4% annual growth rate[33]
Ethylene	CN	21	[36]	Governmental organization	
	EU	18	[37]	Regional industrial association	
	IN	7	[38]	Regional industrial association	
	JP	6	[39]	Governmental organization	
	KR	9	[40]	Governmental organization	
	RAF	2	[41]	Market insight report	
	RME	32	[42, 43]	Own estimation	Estimated with regional capacity (from market insight report[42]) and capacity utilization (from regional industrial association[43])
	RU	3	[44]	Market insight report	Unknown reporting year
	US	31	[45]	Market insight report	
	RoW	35		Own estimation	Difference of global and regional production volumes
	GLO	164	[46]	Market insight report	
Propylene	CN	32	[47]	Market insight report	
	EU	13	[37]	Regional industrial association	
	IN	6	[38]	Regional industrial association	
	JP	6	[39]	Governmental organization	
	KR	8	[40]	Governmental organization	
	RAF	6	[48]	Market insight report	
	RME	10	[43, 49]	Own estimation	Estimated with regional capacity (from market insight report[49]) and capacity utilization (from regional industrial association[43])
	RU	2	[48]	Market insight report	
	US	16	[45]	Market insight report	
	RoW	15		Own estimation	Difference of global and regional production volumes
	GLO	114	[50]	Market insight report	

Benzene, toluene, xylene (BTX)	CN	28	51, 52	Own estimation	Extrapolated from benzene[51] and para-xylene[52] production volume with a factor of 1.19, according to according to the global material flow analysis for the year 2013.[53]
	EU	11	37, 54	Own estimation	Extrapolated from 2015 BTX production volume[54] and production growth rate of benzene [37]
	IN	6	34	Governmental organization	
	JP	10	39	Governmental organization	
	KR	22	40	Governmental organization	
	RAF	1		Own estimation	See description below
	RME	17		Own estimation	Estimated with regional capacity (from market insight report[42]) and capacity utilization (from regional industrial association[43])
	RU	3		Own estimation	See description below
	US	11	45	Own estimation	Extrapolated from benzene and para-xylene production volume[45] with a factor of 1.19, according to according to the global material flow analysis for the year 2013.[53]
	RoW	3		Own estimation	Difference of global and regional production volumes
	GLO	111	49	Own estimation	Extrapolated from benzene and para-xylene production volume[49] with a factor of 1.19, according to according to the global material flow analysis for the year 2013.[53] Extrapolated from 2017 demand volume, assuming 3.4% annual growth rate[49]

* excluding intermediate use for ethylene / propylene production

Due to data scarcity, the total BTX production in Russia Federation and Africa was estimated using the following method:

BTX aromatics are produced either as by-products during the steam cracking, or as by-products in refineries. The production volumes from the two routes were calculated or gathered separately as described below.

Steam cracking: during steam cracking, different feeds would yield different proportions of chemicals. For example, during ethane cracking, the typical yield of ethylene is 0.803, with no BTX produced. However, when naphtha is fed into steam crackers, the typical yields of ethylene and aromatics are 0.324 and 0.103, respectively.[53]

Hence, the regional production of BTX aromatics from steam crackers in Russia Federation and Africa was calculated based on their respective percentage of naphtha, ethane, and other types of feeds used in steam crackers according to the literature (Table S32),[55] in conjunction with the typical yields of ethylene and aromatics from each feed, and regional ethylene production (Table S31), as in Eqn (9). As the exact compositions of other types of feeds are unknown, we assumed that they would yield the same share of products as naphtha.

$$P_{BTX} = P_{ethylene} \times \frac{0.103(f_{naphtha} + f_{other})}{0.324(f_{naphtha} + f_{other}) + 0.803 f_{ethane}} \tag{9}$$

P_{BTX}: estimated production volume of BTX aromatics from steam crackers at a certain region;

$P_{ethylene}$: production volume of ethylene at a certain region;

$f_{naphtha}$, f_{ethane}, and f_{other}: fractions of naphtha, ethane, and other types of oil fed into steam crackers at a certain region, respectively.

Table S32 Feedstock mix in steam crackers, by region, derived from IEA[55]

	$f_{naphtha}$	f_{ethane}	f_{other}
RU	71%	8%	22%
RAF	37%	34%	29%

Refinery: regional BTX production volumes in refineries in Eurasia and Africa were reported for the year of 2017.[55] Eurasia was used as a proxy for Russia Federation due to data constraint. The values were then extrapolated to the year of 2019, assuming an annual growth rate of 3.4% according to Deloitte.[49]

Table S33 Chemical production annual growth, from 2019 to 2050 under the high-emission scenario, by chemical and region

Chemicals	Region	Annual growth	Data source	Note
Urea	CN	-0.3%	55	Urea production stagnated in China in the past decade[36] as a mitigation measure to reduce fertilizer over-application. Hence, the growth rate was assumed to be the same as in the EU, where ammonia production was forecast to slightly decrease
	EU	-0.3%	55	The growth rate of ammonia was used as proxy
	IN	4.0%	56	
	JP	-0.3%	55	The growth rate was assumed to be the same as in the EU due to the similarities in the population and economic growth projections of the two regions
	KR	No production		
	RAF	2.8%	55	The growth rate of ammonia was used as proxy
	RME	2.6%	55	The growth rate of ammonia was used as proxy
	RU	0.6%	55	The growth rate of ammonia in Eurasia was used as proxy
	US	0.9%	55	The growth rate of ammonia in North America was used as proxy
	GLO	1.0%		The growth rate of ammonia was used as proxy
Methanol	CN	2.1%	55	The growth rate of methanol in Asia Pacific was used as proxy
	EU	0.4%	55	
	IN	5.4%	55	The growth rate was assumed to be the same in RAF
	JP	No production		
	KR	No production		
	RAF	5.4%	55	
	RME	1.1%	55	
	RU	4.8%	55	The growth rate of methanol in Eurasia was used as proxy
	US	4.4%	55	The growth rate of methanol in North America was used as proxy

	GLO	2.5%	[55]	
Ethylene / Propylene / BTX aromatics	CN	2.1%	[55]	The growth rate of HVC* in Asia Pacific was used as proxy
	EU	-0.9%	[55]	The growth rate of HVC, negative growth rate due to the accelerated recycling of plastics set by IEA[55]
	IN	7.9%	[55]	The growth rate was assumed to be the same in RAF
	JP	-0.9%	[55]	The growth rate was assumed to be the same in EU, due to the potential similar policies on accelerating plastics recycling
	KR	-0.9%	[55]	The growth rate was assumed to be the same in EU, due to the potential similar policies on accelerating plastics recycling
	RAF	7.9%	[55]	The growth rate of HVC
	RME	4.3%	[55]	The growth rate of HVC
	RU	3.4%	[55]	The growth rate of HVC in Eurasia was used as proxy
	US	1.1%	[55]	The growth rate of HVC in North America was used as proxy
	GLO	1.8%	[55]	The growth rate of HVC

* HVC – high value chemicals, including ethylene, propylene, benzene, toluene, and xylenes.

Table S34 Chemical production annual growth, from 2019 to 2050 under the low-emission scenario, by chemical and region

Chemicals	Region	Annual growth	Data source	Note
Urea	CN	-1.2%	[57]	The growth rate of nitrogen fertilizer with optimized application rate in 2050, same for other regions
	EU	-0.7%	[57]	
	IN	-0.6%	[57]	
	JP	0.0%	[57]	The growth rate in “other OECD countries” was used as proxy
	KR	0.0%	[57]	The growth rate in “other OECD countries” was used as proxy
	RAF	4.0%	[57]	The growth rate in “Sub-Saharan Africa” was used as proxy
	RME	0.0%	[57]	The growth rate in “Middle East and North Africa” was used as proxy
	RU	0.8%	[57]	The growth rate in “Former Soviet Union” was used as proxy
	US	-0.2%	[57]	The growth rate in “USA and Canada” was used as proxy
	GLO	-0.2%	[57]	
Methanol	CN	5.0%	[58]	The production volume was assumed to be 1.53 times of the production volume under the high emission scenario (See GLO for detailed explanation). Same assumptions for other regions, if not otherwise specified.
	EU	2.3%	[58]	
	IN	10.1%	[58]	
	JP	No production	[58]	
	KR	No production	[58]	
	RAF	10.1%	[58]	
	RME	3.3%	[58]	
	RU	9.1%	[58]	
	US	8.4%	[58]	
	GLO	5.6%	[58]	Global methanol production in 2050 under 1.5°C scenario would increase to 224 Mt, due to its potential application as e.g., low-carbon shipping fuel.[58] This number excludes methanol demand in methanol-to-olefins (MTO) / methanol-to-aromatics (MTA) sectors to avoid double counting of CO_2 demand, as the

				demand from MTO and MTA was counted in ethylene, propylene, and BTX aromatics. This is 1.53 times of the production volume under the high-emission scenario (Table S33). The same ratio was taken for regional projections
Ethylene / Propylene / BTX aromatics	CN	-0.3%	[13]	45% of raw materials for plastic can be saved through reuse and mechanical recycling.[13] As the majority of HVCs are further processed into plastics, the growth rate was calculated based on the assumption that the production would be 45% less than under the high-emission scenario in 2050. Same assumptions for other regions, if not otherwise specified
	EU	-1.5%	[13]	Since accelerated recycling was already into account in the modeling of the high-emission scenario, the 45% reduction potential was assumed to be based on the production volume in 2019 to avoid double counting the reduction potential.
	IN	2.9%	[13]	
	JP	-1.5%	[13]	The growth rate was assumed to be the same in EU
	KR	-1.5%	[13]	The growth rate was assumed to be the same in EU
	RAF	2.9%	[13]	
	RME	0.9%	[13]	
	RU	0.4%	[13]	
	US	-0.9%	[13]	
	GLO	-0.3%	[13]	

S1.2.2 CO_2-based production routes

The CO_2-based production routes of the seven key chemicals and their corresponding specific CO_2-feedstock needs were summarized in Table S35.

Table S35 CO_2-based production routes of key chemicals

Chemicals	CO_2-based production routes	Specific CO_2 demand (kg CO_2/kg chemical)	Technology Readiness Level (TRL)
1. Urea	Reaction of CO_2 and ammonia, same as existing processes	0.75	9
2. Methanol	Direct hydrogenation of CO_2	1.39	7
3. Ethylene	Methanol-to-olefins (MTO)	3.61	9
4. Propylene	Methanol-to-olefins (MTO)	3.61	9
5-7. BTX aromatics	Methanol-to-aromatics (MTA)	5.98	7

Chemical 1: ammonia and urea. Ammonia was assumed to be produced with the Haber-Bosch process, with hydrogen coming from water electrolysis. The production of 1 kg of ammonia would require 0.178 kg of hydrogen.[59] Around 55% of ammonia is further processed into urea worldwide today, consuming CO_2 as feedstock. This production pathway was commercialized and was assumed to stay the same in 2050. Assuming a conversion rate of 97.7%,[53] 1 kg of urea would require 0.75 kg of CO_2 stoichiometrically.

Chemical 2: methanol. Conventionally, methanol is produced from fossil fuel-based synthesis gas (syngas). The CO_2-based methanol production assumed in this study was based on the principle of direct hydrogenation of CO_2, using low-carbon hydrogen and CO_2 sourced from carbon capture as feedstocks. This production pathway reached a TRL of 7.[59] Based on a 99.0%

conversion rate,[53] specific CO_2 and H_2 demand for methanol production was calculated to be 1.39 kg CO_2 and 0.189 kg H_2/kg CH_3OH.

Chemical 3 and 4: ethylene and propylene. Light olefins can be produced with the commercialized methanol-to-olefin (MTO) process. The process is widely adopted in China today, with methanol mainly produced from coal.[60] Therefore, MTO route has a TRL of 9. CO_2-based methanol was assumed to be utilized for ethylene and propylene production in this study. 2.83 kg methanol is required to produce 1 kg of ethylene or propylene.[59] This was translated into 3.93 kg specific CO_2 demand and 0.535 kg specific H_2 demand.

Chemical 5-7: benzene, toluene, and xylene (BTX). The methanol-to-aromatics (MTA) route was assumed to be the main production route for BTX in a CO_2-based chemical industry. The process was reported to have a TRL of 7, with total BTX yield of 56%.[59] This means 4.3 kg methanol is required to produce 1 kg of BTX.[59] Ultimately, 5.98 kg CO_2 and 1.13 kg H_2 is needed to produce 1 kg of BTX. Due to data constraint, we did not differentiate the yield difference among BTX.

S1.2.3 Quantifying CO_2-feedstock demand in the chemical industry in 2050

With the projection of the regional production volume of P_i (in Megatonne (MT)/year) of each primary chemical i and its corresponding specific CO_2 demand SCD_i, the total regional CO_2 demand (TCD) can be calculated with Eqn (10), assuming all seven primary chemicals are exclusively produced via CO_2-based routes.

$$TCD = \sum_i P_i \times SCD_i \tag{10}$$

The calculated regional CO_2 demand in 2050 as feedstock per key chemical was summarized in under high- and low-emission scenarios (Table S36).

Table S36 CO_2 demand in 2050 as chemical feedstocks, by scenario, chemical and region

Chemicals	Region	CO_2 demand in 2050 (Mt/year)	
		High-emission scenario	Low-emission scenario
Urea	CN	37	26
	EU	6	5
	IN	41	15
	JP	0	0
	KR	0	0
	RAF	16	19
	RME	31	17
	RU	8	8
	US	9	7
	RoW	25	27
	GLO	174	124
Methanol	CN	83	127
	EU	5	7
	IN	1	2

	JP	0	0
	KR	0	0
	RAF	10	15
	RME	27	42
	RU	16	24
	US	19	29
	RoW	43	66
	GLO	203	311
Ethylene	CN	123	68
	EU	49	37
	IN	85	47
	JP	17	13
	KR	24	18
	RAF	22	12
	RME	266	147
	RU	23	13
	US	152	83
	RoW	170	93
	GLO	930	529
Propylene	CN	192	129
	EU	35	26
	IN	70	45
	JP	15	11
	KR	22	17
	RAF	76	51
	RME	82	57
	RU	17	11
	US	75	37
	RoW	62	73
	GLO	647	458
Benzene, toluene, xylene (BTX)	CN	275	185
	EU	49	37
	IN	119	77
	JP	44	33
	KR	97	72
	RAF	11	7
	RME	229	160
	RU	33	22
	US	89	43
	RoW	94	26
	GLO	1039	662
Total CO_2 demand	CN	710	536
	EU	145	112
	IN	317	185

(sum of above)	JP	75	56
	KR	143	107
	RAF	134	104
	RME	636	423
	RU	97	78
	US	344	199
	RoW	393	285
	GLO	2993	2085

S1.3 Environmental impacts of carbon capture

S1.3.1 Energy need for capturing 1 kg CO_2 from different industries

A simplified flowsheet of carbon capture with chemical absorption is shown in Fig. S1.

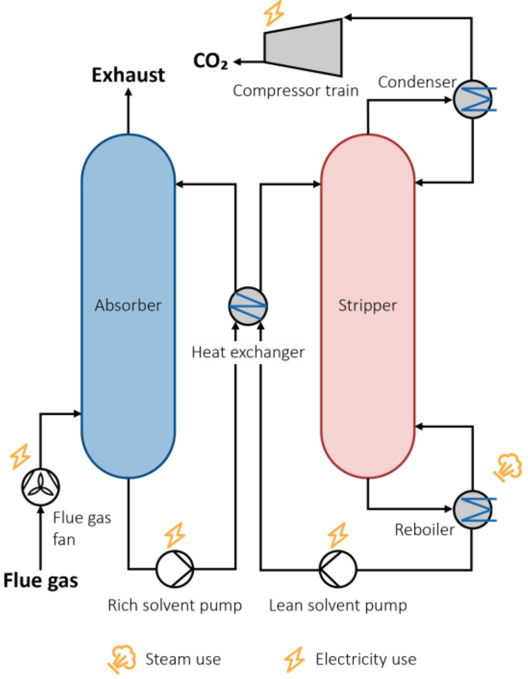


Fig. S1 Simplified flowsheet of carbon capture with chemical absorption

The additional steam and electricity need for carbon capture was obtained by comparing the system with and without carbon capture. Table S37 summarizes the additional energy need due to carbon capture for different industries and explains the corresponding systems with and without carbon capture.

Table S37 Additional fuel and electricity need for capturing 1 kg CO_2 with 90% capture rate from different sectors

	Additional steam (MJ/kg CO_2)	Additional electricity (kWh/kg CO_2)	Note	Data source
Power, coal / solid biomass	0	0.34	The same fuel input was assumed for the cases with and without carbon capture. The decrease in net power output due to carbon capture was set to be compensated by the	[62]

Power, natural gas	0	0.54	grid. This assumption is in line with the existing carbon capture project at Boundary Dam coal-fired power plant.[61]	
Steel, BF-BOF	0.68	0.36	Carbon capture was assumed to be performed for flue gases from the steam boiler, the hot stoves, the coke plant, and the lime plant (72% of the total CO$_2$ emissions of the integrated steel mill). In the reference steel mill without carbon capture, the steam need is satisfied with BOF waste heat boilers, and the electricity need of the integrated mill is partially satisfied by blast furnace gas (BFG) and basic oxygen furnace gas (BOFG). In addition, 76 kWh electricity/tonne steel was assumed to be supplied from the grid. With carbon capture, the site was assumed to be modified so that BFG and BOFG are used to generate steam for MEA regeneration (2.27 MJ steam/kg CO$_2$ captured) prior to the use of additional fuel. All electricity need (622 kWh/tonne steel) was set to be supplied by the grid. Hence the additional electricity need for carbon capture was calculated as 622-76=546 kWh/tonne steel produced. Considering 1.53 tonne CO$_2$ capture per tonne steel produced, the additional electricity need for carbon capture became 0.36 kWh/kg CO$_2$ captured.	63
Steel, DRI-EAF	3.48	0.17	Due to data constraint, the same steam and electricity consumption was assumed as capturing from cement kilns, due to the similar CO$_2$ concentration in flue gas from DRI-EAF steel mills and cement kilns (20vol% on the dry basis).[64, 65]	
Steel, SR-BOF	0	0.15	The HIsarna process was assumed as a typical SR-BOF process, where pure oxygen is fed into the reactor.[66] Assuming pure CO$_2$ in flue gas, the only additional energy required for carbon capture is the electricity need (0.15 kWh/kg CO$_2$ captured)[64] for compressing CO$_2$ to 110 bar for transportation.	
Cement	2.95	0.17	3.48 MJ/kg CO$_2$ steam is required for MEA regeneration.[64] 583 MJ waste heat per tonne clinker production was assumed to be recovered for energy use.[67] This value was obtained using an average heat input of 3610 MJ/tonne clinker, and due to data constraints, was used in all regions under both scenarios regardless of the regional average heat input. This was a generous assumption, because with the improvement in energy efficiency by 2050, the amount of waste heat available would be expected to decrease. Steam need for the MEA regeneration was assumed to be supplied by waste heat prior to use of additional fuel. The availability of waste heat was therefore deducted when calculating the additional steam need.	64
Kraft pulp	0	0.37	Carbon capture was assumed to be performed for flue gases from the recovery boiler, the multi-fuel boiler, and the lime kiln. Kraft pulp mills are net electricity exporters both with and without carbon capture. Therefore, the system is similar to power plants. The same fuel input was assumed for the cases with and without carbon capture. The decrease in net power output due to carbon capture was set to be compensated by the grid.	26

S1.3.2 Environmental impacts of the electricity grid mix

S1.3.2.1 Climate change impacts of the electricity grid mix

Life cycle assessment (LCA) was performed for the regional electricity grid mix in 2019 and in 2050 under four different scenarios (high-emission scenario without carbon capture, utilization or storage (CCUS), high-emission scenario with full CCUS deployment, low-emission scenario without CCUS, and low-emission scenario with full CCUS deployment). For scenarios with full CCUS deployment, 90% CO_2 capture was assumed to be performed at coal-, natural gas-, and solid biomass-fired power plants.

Ecoinvent 3.8[68] was used as a basis for the life cycle inventories (LCIs) of the regionalized electricity grid mix. As the first step, fuel type match was performed to link all the high voltage electricity generation datasets used in the regional electricity grid mixes (high-voltage) in the ecoinvent database with different electricity generation types as in the "*Extended World Energy Balances*" in IEA's *World Energy Statistics and Balances*.[7] The dataset match is listed in Table S38. For electricity generation from photovoltaic power stations, it is only possible to feed into medium- or high-voltage grid if the capacity is in the higher kilowatt to megawatt range. However, the future design and sizes of photovoltaic power stations remain uncertain.[69] Ecoinvent assumes that electricity generation from photovoltaic modules feeds into the low voltage grid mix, whilst industries typically use electricity from the median voltage grid mix.[70] This assumption was also applied in 2050 scenarios.

Table S38 Match of high voltage electricity generation datasets in ecoinvent 3.8 with the electricity generation types

Electricity type	Dataset name as in ecoinvent 3.8, with reference product as "electricity, high voltage"
Coal	'electricity production, hard coal', 'electricity production, hard coal, conventional', 'electricity production, hard coal, supercritical', 'electricity production, lignite', 'electricity production, peat', 'heat and power co-generation, hard coal', 'heat and power co-generation, lignite'
Oil	'electricity production, oil', 'heat and power co-generation, diesel, 200kW electrical, SCR-NOx reduction', 'heat and power co-generation, oil'
Natural gas	'electricity production, natural gas, 10MW', 'electricity production, natural gas, combined cycle power plant', 'electricity production, natural gas, conventional power plant', 'heat and power co-generation, natural gas, 1MW electrical, lean burn', 'heat and power co-generation, natural gas, 200kW electrical, lean burn', 'heat and power co-generation, natural gas, 500kW electrical, lean burn', 'heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical', 'heat and power co-generation, natural gas, conventional power plant, 100MW electrical'
Nuclear	'electricity production, nuclear, boiling water reactor' 'electricity production, nuclear, pressure water reactor', 'electricity production, nuclear, pressure water reactor, heavy water moderated'
Solid biomass	'heat and power co-generation, wood chips, 2000 kW', 'heat and power co-generation, wood chips, 2000 kW, state-of-the-art 2014', 'heat and power co-generation, wood chips, 6667 kW', 'heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014'
Biogas	'heat and power co-generation, biogas, gas engine'
Hydro	'electricity production, hydro, reservoir, alpine region',

	'electricity production, hydro, reservoir, non-alpine region', 'electricity production, hydro, reservoir, tropical region', 'electricity production, hydro, run-of-river'
Wind	'electricity production, wind, 1-3MW turbine, offshore', 'electricity production, wind, 1-3MW turbine, onshore', 'electricity production, wind, <1MW turbine, onshore', 'electricity production, wind, >3MW turbine, onshore'
Other renewables	'electricity production, deep geothermal', 'electricity production, solar thermal parabolic trough, 50 MW', 'electricity production, solar tower power plant, 20 MW'

With the Brightway2 framework[71] and the Wurst package,[72] the ecoinvent datasets were modified as following:

1. The regional electricity grid mix (high voltage) was updated according to descriptions in Section S1.1.1.1 for 2019, 2050 high-emission scenario and 2050-low-emission scenario (Table S39).

Table S39 High voltage electricity grid mix, by scenario and region

Scenario	Region	High voltage electricity grid mix							
		Coal	Oil	Natural gas	Nuclear	Solid biomass	Biogas	Hydro	Wind
2019	CN	68%	0%	3%	5%	0%	0%	18%	6%
	EU	16%	1%	19%	31%	3%	2%	12%	16%
	IN	72%	0%	3%	4%	0%	0%	15%	5%
	JP	32%	2%	44%	9%	2%	0%	10%	1%
	KR	40%	1%	27%	30%	1%	0%	1%	1%
	RAF	31%	8%	40%	2%	0%	0%	18%	2%
	RME	0%	14%	81%	1%	0%	0%	3%	0%
	RU	17%	0%	44%	20%	0%	0%	19%	0%
	US	26%	0%	37%	22%	0%	0%	7%	8%
	RoW	23%	6%	25%	6%	0%	0%	35%	4%
	GLO	38%	2%	23%	12%	0%	0%	18%	6%
2050 high-emission scenario	CN	33%	0%	5%	12%	3%	2%	18%	26%
	EU	1%	0%	12%	17%	6%	4%	15%	45%
	IN	33%	0%	6%	10%	0%	5%	13%	33%
	JP	7%	8%	16%	22%	10%	0%	13%	24%
	KR	0%	0%	50%	19%	6%	1%	0%	24%
	RAF	9%	3%	37%	3%	3%	0%	25%	19%
	RME	1%	8%	69%	5%	0%	2%	2%	13%
	RU	9%	0%	44%	19%	2%	1%	18%	7%
	US	1%	0%	40%	14%	2%	2%	10%	31%
	RoW	15%	0%	25%	5%	4%	1%	31%	19%
	GLO	17%	1%	23%	10%	3%	2%	19%	25%
2050 low-emission scenario	CN	4%	0%	2%	15%	5%	3%	19%	52%
	EU	0%	0%	0%	13%	6%	4%	9%	67%
	IN	2%	0%	1%	10%	0%	11%	13%	62%

JP	3%	1%	3%	28%	12%	0%	13%	40%
KR	0%	0%	25%	14%	9%	1%	0%	51%
RAF	1%	0%	3%	5%	7%	0%	32%	51%
RME	0%	0%	6%	9%	0%	3%	3%	78%
RU	0%	0%	4%	33%	10%	6%	27%	21%
US	1%	0%	1%	16%	4%	3%	7%	67%
RoW	0%	0%	1%	6%	7%	1%	34%	51%
GLO	1%	0%	2%	12%	6%	3%	19%	56%

2. For all coal-, oil-, natural gas-, solid biomass-, and biogas-fired electricity production datasets, the foreground CO_2 emissions (in kg CO_2 per kWh) and fuel input (in kg fuel per kWh for coal-, oil-, and solid biomass-, and m^3 per kWh for natural gas and biogas-fired electricity) were updated. The calculations were performed based on regionalized power efficiency of non-CHP power plants (described in Section S1.1.1.2 for 2019, and 2050 high- and low-emission scenarios without CCUS). In the case of CHP power plants, the fuel inputs and emissions were allocated between heat and electricity output with the ratio of 1:2.5 (1 MJ heat : 1 MJ electricity).[73] The apparent electrical efficiency was then calculated with the allocated fuel inputs per unit electricity output. For 2050 scenarios with full CCUS deployment (90% capture rate from the flue gas of coal-, natural gas-, and solid biomass-fired power plants), the updated power efficiency of those power plants was calculated with Eqn. (11).

$$\eta_{with\ CCS} = \eta_{without\ CCUS} - \frac{ELE_{CCUS} \times EF_{fuel} \times 3.6 \times 90\%}{1000} \qquad (11)$$

Where $\eta_{without\ CCUS}$ stands for the apparent power efficiency in the base case without carbon capture (described in Section S1.1.1.2); ELE_{CCUS} is the power loss due to carbon capture (in kWh/kg CO_2 captured, see Table S37), EF_{fuel} is the emission factor of the fuel (in tonne CO_2/TJ fuel, see Table S14). The updated regionalized apparent electrical efficiency was summarized in Table S40. Since no carbon capture was assumed to be performed at oil- or biogas-fired power plants, the power efficiency was set to be the same in scenarios without and with CCUS deployment.

Table S40 Apparent electrical efficiency, by fuel type, scenario and region

Scenario	Region	Apparent electrical efficiency				
		Coal	Oil	Natural gas	Solid biomass	Biogas
2019	CN	38%	36%	53%		43%
	EU	39%	37%	53%	40%	48%
	IN	35%	27%	41%		33%
	JP	41%	32%	52%	38%	46%
	KR	39%	38%	53%	38%	41%
	RAF	32%	19%	40%	28%	40%
	RME	37%	33%	41%		46%
	RU	41%	41%	42%		43%
	US	37%	38%	50%	28%	32%

	RoW	35%	44%	47%	23%	36%
	GLO	37%	27%	47%	35%	43%
2050 high-emission scenario, no CCUS deployment	CN	44%	42%	55%	38%	44%
	EU	45%	42%	58%	40%	54%
	IN	40%	28%	47%	38%	37%
	JP	46%	37%	59%	38%	51%
	KR	45%	28%	59%	38%	46%
	RAF	37%	21%	46%	33%	45%
	RME	43%	38%	47%	38%	52%
	RU	47%	44%	48%	38%	44%
	US	43%	44%	57%	31%	37%
	RoW	40%	44%	54%	27%	41%
	GLO	43%	28%	54%	38%	44%
2050 high-emission scenario, full CCUS deployment	CN	33%	42%	45%	28%	44%
	EU	35%	42%	48%	29%	54%
	IN	30%	28%	38%	27%	37%
	JP	36%	37%	49%	27%	51%
	KR	32%	28%	49%	27%	46%
	RAF	27%	21%	37%	22%	45%
	RME	32%	38%	37%	27%	52%
	RU	37%	44%	39%	28%	44%
	US	32%	44%	48%	20%	37%
	RoW	30%	44%	45%	16%	41%
	GLO	32%	28%	44%	27%	44%
2050 low-emission scenario, no CCUS deployment	CN	47%	44%	55%	39%	59%
	EU	47%	45%	58%	40%	59%
	IN	46%	44%	61%	39%	59%
	JP	46%	44%	61%	38%	59%
	KR	46%	44%	59%	38%	58%
	RAF	46%	44%	61%	39%	59%
	RME	46%	44%	61%	39%	59%
	RU	46%	44%	52%	39%	59%
	US	46%	44%	60%	39%	60%
	RoW	46%	44%	60%	38%	59%
	GLO	47%	44%	58%	39%	59%
2050 low-emission scenario, full CCUS deployment	CN	37%	44%	45%	28%	59%
	EU	36%	45%	48%	29%	59%
	IN	36%	44%	51%	28%	59%
	JP	36%	44%	51%	27%	59%
	KR	36%	44%	49%	27%	58%
	RAF	36%	44%	51%	28%	59%
	RME	36%	44%	51%	28%	59%
	RU	36%	44%	42%	28%	59%
	US	36%	44%	50%	28%	60%

RoW	35%	44%	50%	27%	59%
GLO	36%	44%	49%	28%	59%

The calculation of fuel input (in kg/kWh or m^3/kWh) was performed by taking the net calorific values of fuels (in MJ/kg fuel for coal, oil, and solid biomass, and MJ/m^3 for natural gas and biogas) into account. The net calorific values of each coal and oil product is reported in the "*World conversion factors*" in IEA's *World Energy Statistics and Balances* by country.[7] The weighted regional average of net calorific value of coal and oil was calculated by using the corresponding fuel input to "main activity producer electricity plants" and "main activity producer CHP plants" (in TJ) as weight, which was reported in the "*Extended world energy balances*" in IEA's *World Energy Statistics and Balances* by country.[7] The products categorized into coal and oil were summarized in Table S41. And the derived regionalized calorific values of coal and oil were summarized in Table S42. Ecoinvent reported the net calorific values of high pressure natural gas and biogas to be 39 and 23 MJ/m^3, respectively.[68] For solid biomass, 12.5 MJ/kg calorific value of wood chips with 30% moisture (equivalent to 18 MJ/kg on the dry mass) reported by Forest Research[74] was used in this study. Due to a lack of regionalized data, those values were used for all regions.

Table S41 Products by fuel type (coal and oil)

Fuel type	Products as in *World conversion factors* and *Extended world energy balances*[7]
Coal	anthracite, coking coal, other bituminous coal, sub-bituminous coal, lignite, BKB, oil shale and oil sands, petroleum coke, coke oven coke, peat, peat products
Oil	crude oil, kerosene type jet fuel excl. biofuels, gas/diesel oil excl. biofuels, fuel oil, naphtha, bitumen, other oil products

Table S42 Weighted average calorific values of coal and oil, by region

Region	Weighted average calorific values (MJ/kg)	
	Coal	Oil
CN	21	42
EU	12	41
IN	17	42
JP	25	41
KR	23	43
RAF	23	41
RME	20	42
RU	20	40
US	21	41
RoW	18	42
GLO	20	42

The foreground CO_2 emissions were then calculated with Eqn. (2). The climate change effect of biogenic carbon is closely related to the rotation period of the biomass. Assuming the primary solid biomass is harvested directly from managed forests that have an average rotation period of 90 years for energy generation,[75] a Global Warming Potential (GWP100) of 0.39 kg CO_2-eq. was assigned to one kilogram of biogenic CO_2 emission from solid biomass.[76]

The final updated fuel inputs into power plants and the corresponding CO_2 emissions under different scenarios are summarized in Table S43 and Table S44.

Table S43 Updated fuel input into power plants, by fuel type, scenario and region

Scenario	Region	Fuel inputs Coal (kg/kWh)	Oil (kg/kWh)	Natural gas (m^3/kWh)	Solid biomass (kg/kWh)	Biogas (m^3/kWh)
2019	CN	0.45	0.24	0.17	0.57	0.37
	EU	0.75	0.22	0.17	0.51	0.33
	IN	0.62	0.23	0.22	0.57	0.48
	JP	0.35	0.27	0.18	0.53	0.35
	KR	0.40	0.22	0.17	0.52	0.39
	RAF	0.49	0.26	0.23	0.71	0.34
	RME	0.50	0.46	0.23	0.57	0.40
	RU	0.45	0.33	0.22	0.57	0.37
	US	0.46	0.23	0.18	0.73	0.50
	RoW	0.57	0.20	0.20	0.86	0.44
	GLO	0.49	0.32	0.20	0.57	0.37
2050 high-emission scenario, no CCUS deployment	CN	0.39	0.20	0.17	0.51	0.36
	EU	0.65	0.21	0.16	0.50	0.29
	IN	0.54	0.30	0.20	0.53	0.42
	JP	0.31	0.24	0.16	0.53	0.31
	KR	0.36	0.30	0.16	0.53	0.34
	RAF	0.43	0.23	0.20	0.62	0.30
	RME	0.43	0.40	0.20	0.53	0.35
	RU	0.39	0.20	0.19	0.51	0.36
	US	0.40	0.20	0.16	0.64	0.43
	RoW	0.50	0.20	0.17	0.75	0.39
	GLO	0.43	0.31	0.17	0.53	0.36
2050 high-emission scenario, full CCUS deployment	CN	0.51	0.20	0.20	0.71	0.36
	EU	0.86	0.21	0.19	0.69	0.29
	IN	0.72	0.30	0.25	0.74	0.42
	JP	0.40	0.24	0.19	0.74	0.31
	KR	0.57	0.30	0.19	0.74	0.34
	RAF	0.59	0.23	0.25	0.92	0.30
	RME	0.57	0.40	0.25	0.74	0.35
	RU	0.50	0.20	0.24	0.71	0.36
	US	0.53	0.20	0.19	0.99	0.43
	RoW	0.67	0.20	0.21	1.27	0.39
	GLO	0.57	0.31	0.21	0.74	0.36
2050 low-emission scenario, no CCUS deployment	CN	0.36	0.20	0.17	0.51	0.27
	EU	0.63	0.20	0.16	0.50	0.27
	IN	0.47	0.19	0.15	0.52	0.27
	JP	0.31	0.20	0.15	0.53	0.27

	KR	0.33	0.19	0.16	0.53	0.27
	RAF	0.35	0.20	0.15	0.51	0.27
	RME	0.40	0.20	0.15	0.52	0.27
	RU	0.39	0.20	0.18	0.51	0.27
	US	0.37	0.20	0.15	0.52	0.26
	RoW	0.44	0.20	0.15	0.53	0.27
	GLO	0.39	0.20	0.16	0.52	0.27
2050 low-emission scenario, full CCUS deployment	CN	0.46	0.20	0.20	0.71	0.27
	EU	0.82	0.20	0.19	0.69	0.27
	IN	0.61	0.19	0.18	0.72	0.27
	JP	0.40	0.20	0.18	0.74	0.27
	KR	0.43	0.19	0.19	0.74	0.27
	RAF	0.45	0.20	0.18	0.71	0.27
	RME	0.52	0.20	0.18	0.72	0.27
	RU	0.51	0.20	0.22	0.71	0.27
	US	0.48	0.20	0.18	0.72	0.26
	RoW	0.57	0.20	0.18	0.74	0.27
	GLO	0.51	0.20	0.19	0.72	0.27

Table S44 Updated CO_2 emission factors accountable for climate change impacts of electricity production, by fuel type, scenario and region

Scenario	Region	CO_2 emission factors accountable for climate change impacts (kg CO_2-eq./kWh)				
		Coal	Oil	Natural gas	Solid biomass	Biogas
2019	CN	0.89	0.75	0.38	0.40	0
	EU	0.90	0.69	0.38	0.35	0
	IN	0.98	0.73	0.49	0.40	0
	JP	0.83	0.87	0.39	0.37	0
	KR	0.88	0.73	0.38	0.37	0
	RAF	1.05	0.82	0.50	0.49	0
	RME	0.93	1.45	0.50	0.40	0
	RU	0.85	1.02	0.48	0.40	0
	US	0.93	0.72	0.40	0.51	0
	RoW	0.98	0.62	0.43	0.60	0
	GLO	0.92	1.00	0.43	0.40	0
2050 high-emission scenario, no CCUS deployment	CN	0.78	0.65	0.37	0.36	0
	EU	0.78	0.65	0.35	0.35	0
	IN	0.85	0.95	0.43	0.37	0
	JP	0.74	0.75	0.34	0.37	0
	KR	0.80	0.99	0.34	0.37	0
	RAF	0.91	0.72	0.44	0.43	0
	RME	0.81	1.27	0.43	0.37	0
	RU	0.74	0.63	0.42	0.36	0
	US	0.81	0.62	0.35	0.45	0
	RoW	0.86	0.62	0.37	0.52	0

	GLO	0.80	0.97	0.38	0.37	0
2050 high-emission scenario, full CCUS deployment	CN	0.10	0.65	0.04	-0.64	0
	EU	0.10	0.65	0.04	-0.63	0
	IN	0.11	0.95	0.05	-0.68	0
	JP	0.10	0.75	0.04	-0.68	0
	KR	0.11	0.99	0.04	-0.67	0
	RAF	0.13	0.72	0.06	-0.84	0
	RME	0.11	1.27	0.05	-0.68	0
	RU	0.10	0.63	0.05	-0.64	0
	US	0.11	0.62	0.04	-0.90	0
	RoW	0.12	0.62	0.05	-1.16	0
	GLO	0.11	0.97	0.05	-0.68	0
2050 low-emission scenario, no CCUS deployment	CN	0.73	0.62	0.37	0.36	0
	EU	0.76	0.61	0.35	0.35	0
	IN	0.74	0.61	0.33	0.36	0
	JP	0.74	0.64	0.33	0.37	0
	KR	0.73	0.62	0.34	0.37	0
	RAF	0.74	0.62	0.33	0.36	0
	RME	0.75	0.62	0.33	0.36	0
	RU	0.75	0.63	0.39	0.36	0
	US	0.75	0.62	0.34	0.36	0
	RoW	0.76	0.62	0.34	0.37	0
	GLO	0.74	0.62	0.35	0.36	0
2050 low-emission scenario, full CCUS deployment	CN	0.09	0.62	0.04	-0.64	0
	EU	0.10	0.61	0.04	-0.63	0
	IN	0.10	0.61	0.04	-0.66	0
	JP	0.10	0.64	0.04	-0.68	0
	KR	0.09	0.62	0.04	-0.67	0
	RAF	0.10	0.62	0.04	-0.64	0
	RME	0.10	0.62	0.04	-0.66	0
	RU	0.10	0.63	0.05	-0.64	0
	US	0.10	0.62	0.04	-0.66	0
	RoW	0.10	0.62	0.04	-0.67	0
	GLO	0.09	0.62	0.04	-0.66	0

With the aforementioned updates, the climate change impacts of regional electricity grid mix was calculated for various scenarios (Table S45).

Table S45 Modeled climate change impacts of regional high voltage electricity grid, by scenario and region

Region	climate change impacts of high voltage electricity grid mix (kg CO_2-eq./kWh)				
	2019	2050 high-emission scenario, no CCUS deployment	2050 high-emission scenario, full CCUS deployment	2050 low-emission scenario, no CCUS deployment	2050 low-emission scenario, full CCUS deployment
CN	0.825	0.392	0.130	0.088	0.002

EU	0.457	0.212	0.051	0.043	-0.008
IN	0.917	0.408	0.134	0.058	0.041
JP	0.299	0.103	-0.001	0.049	-0.017
KR	0.597	0.261	0.053	0.108	-0.053
RAF	0.474	0.360	0.123	0.111	-0.007
RME	0.532	0.233	0.017	0.147	-0.024
RU	0.633	0.313	0.061	0.066	-0.024
US	0.668	0.452	0.196	0.042	0.023
RoW	0.454	0.307	0.042	0.062	-0.024
GLO	0.589	0.321	0.084	0.067	-0.008

S1.3.2.2 Particulate Matter (PM)-related health impacts of the electricity grid mix

PM-related health impacts of the electricity grid mix was assumed to come from the release of the pollutants such as primary fine particulate matter, sulfur dioxide, nitrogen oxides and ammonia during the combustion of fossil fuels (coal, oil, and natural gas) and biofuels (solid biomass and biogases) onsite the corresponding power plants. The regionalized PM-related impacts factors of fossil-fueled power plants from Oberschelp *et al.* (in DALY/MJ fuel input) calculated from the energy balances and the characterization factors there were used in this study.[77] The impact factors of solid biomass-fueled power plants were calculated with the emission factors of wood with electrostatic precipitators reported in the *Draft Revisions to AP-42 (Compilation of Air Emissions Factors)* from the United States Environmental Protection Agency[78] and the model from Oberschelp *et al.*[79] with the following assumptions: (1) the locations and power generation amount from primary solid biomass were assumed to be the same as for coal-fired power plants; (2) the stack height was assumed to be 50 meter; (3) the flue gas exit velocity was assumed to be 20 meter per second. Due to a lack of data, the impacts factors of biogas-fueled power plants were assumed to be the same as natural gas-fueled power plants. These impacts factors were combined with the power efficiency (Table S40) and the electricity grid mix (Table S39) under different scenarios to derive the PM-related health impacts factors of the regional high voltage electricity grid mix (Table S46).

Table S46 Modeled PM-related health impacts of regional high voltage electricity grid mix, by scenario and region

Region	PM-related health impacts of high voltage electricity grid mix (DALY/kWh)				
	2019	2050 high-emission scenario, no CCUS deployment	2050 high-emission scenario, full CCUS deployment	2050 low-emission scenario, no CCUS deployment	2050 low-emission scenario, full CCUS deployment
CN	1.92E-08	1.15E-08	1.52E-08	6.45E-09	8.68E-09
EU	1.48E-08	4.72E-09	6.17E-09	2.94E-09	3.96E-09
IN	1.90E-07	7.69E-08	1.03E-07	5.07E-09	6.18E-09
JP	1.43E-08	6.26E-09	8.31E-09	5.41E-09	7.33E-09
KR	2.13E-08	2.44E-08	2.96E-08	1.44E-08	1.96E-08
RAF	1.27E-08	7.78E-09	9.92E-09	3.24E-09	4.31E-09
RME	2.25E-08	9.77E-09	1.31E-08	1.17E-08	1.61E-08
RU	4.27E-08	1.58E-08	1.88E-08	2.26E-09	2.90E-09
US	5.00E-08	2.68E-08	2.77E-08	4.76E-10	5.52E-10

RoW	4.23E-08	2.12E-08	2.92E-08	5.90E-09	8.07E-09
GLO	3.38E-08	1.94E-08	2.54E-08	5.21E-09	7.01E-09

S1.3.3 Environmental impacts of steam production

Additional fuel is required to produce steam for carbon capture in cement kilns and steel mills. Different scenarios were assumed for the fuel source:

1) the steam boiler uses the same fuel as the main production activity (this means e.g., coal for BF-BOF steel mills and natural gas for DRI-EAF steel mills), with 90% thermal efficiency;
2) the steam boiler uses only natural gas as fuel, with 90% thermal efficiency;
3) the steam is produced from electrode vessels that uses grid electricity with 99% thermal efficiency.[80]

S1.3.3.1 Climate change impacts of steam production

For climate change impacts, the background datasets of fuel supply from ecoinvent 3.8 were used in this study. Where regional data are missing, the dataset for the Rest of the World (RoW) was used. Table S47 summarizes names and locations of the applied ecoinvent datasets. The foreground greenhouse gas emission factors of fuel combustion were from the *IPCC Guidelines for National Greenhouse Gas Inventories*.[10] The climate change impacts from background processes of fuel supply and foreground processes of fuel combustion was combined with the net calorific values of the fuels (described in Section S1.3.2) and a 90% thermal efficiency of the steam boiler for the GWP calculation of the steam (in kg CO_2-eq./MJ fuel). The results were summarized in

Table S48.

Table S47 Ecoinvent datasets of fuel supply used in this study, by fuel type and region

Fuel	Coal	Oil	Natural gas	Solid biomass
Dataset name as in ecoinvent 3.8	Market for hard coal	Market for heavy fuel oil	Market for natural gas, high pressure	Market for wood chips, wet, measured as dry mass
Regions in this study	Regions of the dataset as in ecoinvent 3.8			
CN	CN	RoW	RoW	RoW
EU	Europe without Russia and Turkey	Europe without Switzerland	RoW	Europe without Switzerland
IN	IN	IN	RoW	RoW
JP	RoW	RoW	JP	RoW
KR	RoW	RoW	RoW	RoW
RAF	RoW	RoW	RoW	RoW
RME	RoW	RoW	RoW	RoW
RU	RU	RoW	RU	RoW
US	RNA	RoW	US	RoW
RoW	RoW	RoW	RoW	RoW

Table S48 Modeled climate change impacts of regional fuel combustion, by fuel type and region

Region	climate change impacts of fuel combustion (kg CO_2-eq./MJ)			
	Coal	Oil	Natural gas	Solid biomass
CN	0.121	0.083	0.063	0.042
EU	0.123	0.083	0.063	0.041
IN	0.110	0.086	0.063	0.042
JP	0.110	0.083	0.075	0.042
KR	0.112	0.083	0.063	0.042
RAF	0.112	0.083	0.063	0.042
RME	0.115	0.083	0.063	0.042
RU	0.111	0.083	0.071	0.042
US	0.104	0.083	0.068	0.042
RoW	0.117	0.083	0.063	0.042

S1.3.3.2 Particulate Matter (PM)-related health impacts of steam production

For PM-related health impacts, only the impacts related to fuel combustion were considered. Other relevant considerations were described in Section S1.3.2.2.

S1.4 Bottom-up case studies: development and application of CO_2-feedstock sourcing strategies in China and Middle East

S1.4.1 Locations and capacities of individual CO_2 suppliers and consumers

Site specific information including latitude, longitude and production capacity were collected for chemical manufacturing sites (as CO_2 consumers) and cement kilns, steel mills, coal- and natural gas-fired power plants (as CO_2 suppliers) were collected from various sources as summarized in Table S49.

Table S49 Data sources of locations and capacities of individual CO_2 suppliers and consumers

	China	Middle East
CO_2 consumers (chemical manufacturing sites)	Manual collection from public available information sources (see Appendix table)	Manual collection from public available information sources (see Appendix table)
CO_2 suppliers		
Cement kilns	Manual collection from public available information sources (see Appendix table)	[77]
Steel mills	[77]	[77, 81]
Coal-fired power plants	[82]	[82]
Natural gas-fired power plants	[83]	[83]

S1.4.2 Elimination strategy of coal-fired power plants in China and natural gas-fired power plants in Middle East

IEA predicted the electricity generation and the corresponding electrical capacity by fuel type and region in its *World Energy Outlook 2020*.[3] With these two factors, the estimated average annual operation hours were calculated to be 2065 hours for coal-fired power plants in China and 2529 hours for natural gas-fired power plants in Middle East under the Sustainable Development Scenario in 2040. Due to a lack of more representative estimations, those two values were assumed to be the average operation hours of the respective power plants under the low-emission scenario in 2050 in this study. As described in Section S1.1.1.1, total electricity generation from coal would be 449 TWh in China and total electricity generation from natural gas would be 124 TWh in Middle East under the low-emission scenario in 2050. The remaining electrical capacity was then back-calculated to be 218 GW coal-fired power plants in China and 49 GW natural gas-fired power plants in Middle East, reducing from 1307 GW coal-fired power plants in China and 316 GW natural gas-fired power plants in Middle East that are in operation, construction, or planning today.[82, 83]

Therefore, a simplified phase-out strategy was developed according to Cui *et al.*[84] to match the abovementioned remaining capacity. Specifically, only technical attributes including age, size, technology, and application as reported by Global Energy Monitor[82, 83] were taken into account. Profitability and Environmental impacts were not considered due to data constraint. However, these two factors are also to a large extent correlated with the technical attributes. A scoring system was designed by Cui *et al.*[84] for coal-fired power plants (Table S50) and was adapted for natural gas-fired power plants (Table S51). The power generation units with higher total scores were set to be kept until the total capacity was reached. The remaining units were assumed to be phased out and were not included in the case study.

Table S50 Score assignment to coal-fired power plants in China, based on Cui et al.[84]

	Data Type	Score Assignment			
Age	Quantitative	[min, max]			
		[0,1]			
Size	Categorical	<300MW	>=300MW	>=600MW	>=1000MW
		0.25	0.5	0.75	1
Technology	Categorical	Other	Subcritical	Supercritical	Ultra-Super
		0.25	0.5	0.75	1
Application	Categorical	Self-Use	CHP	Power	
		0.5	1	1	

Table S51 Score assignment to natural gas-fired power plants in the Middle East

	Data Type	Score Assignment
Age	Quantitative	[min, max]
		[0,1]

Size	Categorical	<200MW	>=200MW	>=400MW	>=600MW
		0.25	0.5	0.75	1
Technology	Categorical	Steam turbine	Gas turbine	Combined cycle	
		0.5	0.75	1	
Application	Categorical	Non-CHP	CHP		
		0.5	1		

S1.4.3 Environmental impacts of truck transportation

Climate change impacts of truck transportation (in kg CO_2-eq. per tonne kilometer) was obtained based on the dataset “transport, freight, lorry 16-32 metric ton, EURO3 | RoW” in ecoinvent 3.8. The inventory from this dataset was then combined with the regionalized characterization factors for ground transport in China and Middle East from Oberschelp *et al.*[79] to calculate the total PM-related health impacts of truck transportation (in DALY per tonne kilometer). The considered inventories include direct emissions of primary particulate matter with a diameter below 2.5 µm ($PM_{2.5}$), sulfur dioxide (SO_2), nitrogen oxides (NO_x), and ammonia (NH_3), and indirect emissions of these substances from road wear, brake wear, and tyre wear.

S1.4.4 Environmental impacts of pipeline transportation

The dataset for CO_2 pipeline transportation was modified based on the dataset for natural gas transportation in ecoinvent 3.8: “market for transport, pipeline, onshore, long distance, natural gas | RoW”. The inventory is shown in Table S52.

Table S52 LCI data of CO_2 transportation with pipeline (1 tonne kilometer)

Technosphere inputs

Amount	Unit	Activity	Location	Comments
2.59E-9	km	Market for pipeline, natural gas, long distance, high capacity, onshore	GLO	Amount from ecoinvent 3.8, proxy for CO_2 pipeline infrastructure
0.0725	kWh	Market group for electricity, medium voltage	CN / RME	Amount from ecoinvent 3.8, electricity need for CO_2 recompression

Biosphere flows

Amount	Unit	Flow name	Compartments	Comments
0.00026	kg	Carbon dioxide, fossil	air	Amount from Wildbolz,[85] CO_2 leakage

S2 Additional results

S2.1 Environmental impacts of carbon capture – sensitivity analysis

Various combinations of electricity grid mix (2019, 2050 without CCUS deployment, 2050 with full CCUS deployment) and steam sources (mixed fuel boilers, natural gas boilers, and electrode vessels) are applied to the Environmental-Merit-Order (EMO) curves of 1 kg CO_2 captured from different industries as part of the sensitivity analysis. The results are shown in Fig. S2 and Fig. S3 for the sectoral rankings in terms of climate change impacts, and Fig. S4 and Fig. S5 for the sectoral rankings in terms of PM-related health impacts.

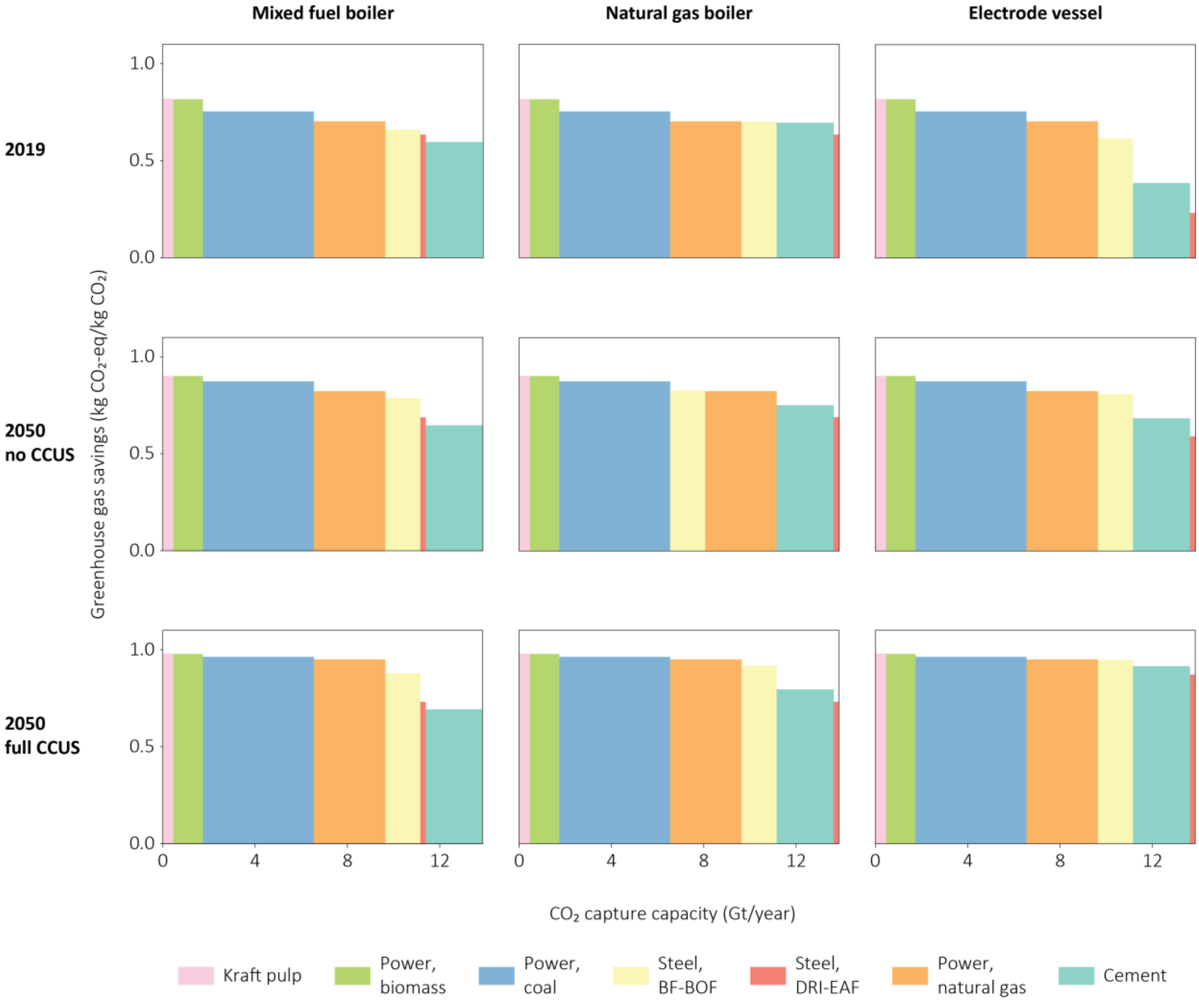


Fig. S2 Environmental-merit-order curve for GHG savings of 1 kg CO_2 captured from different industries under the high-emission scenario with different combinations of electricity and steam sources

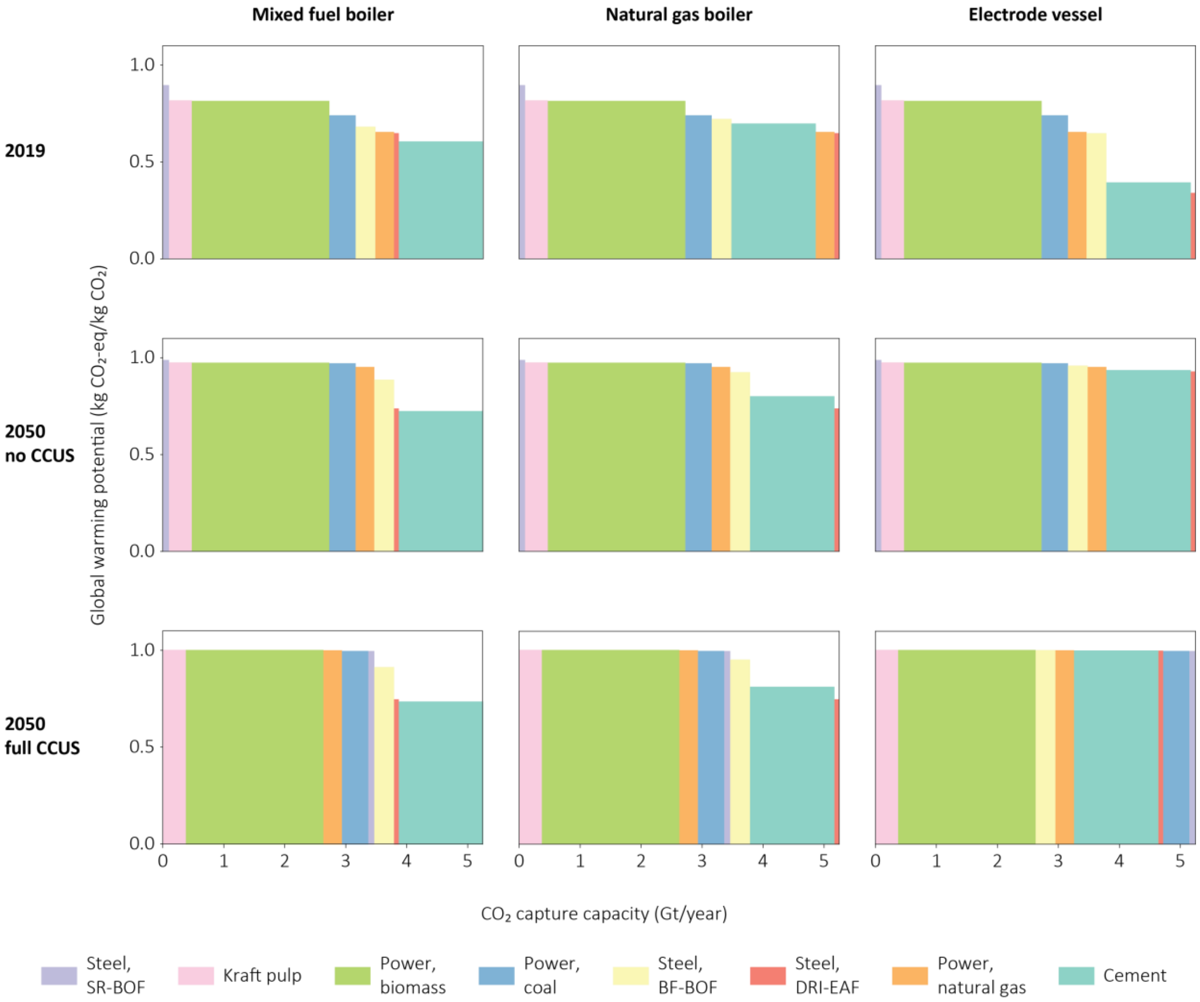


Fig. S3 Environmental-merit-order curve for GHG savings of 1 kg CO_2 captured from different industries under the low-emission scenario with different combinations of electricity and steam sources

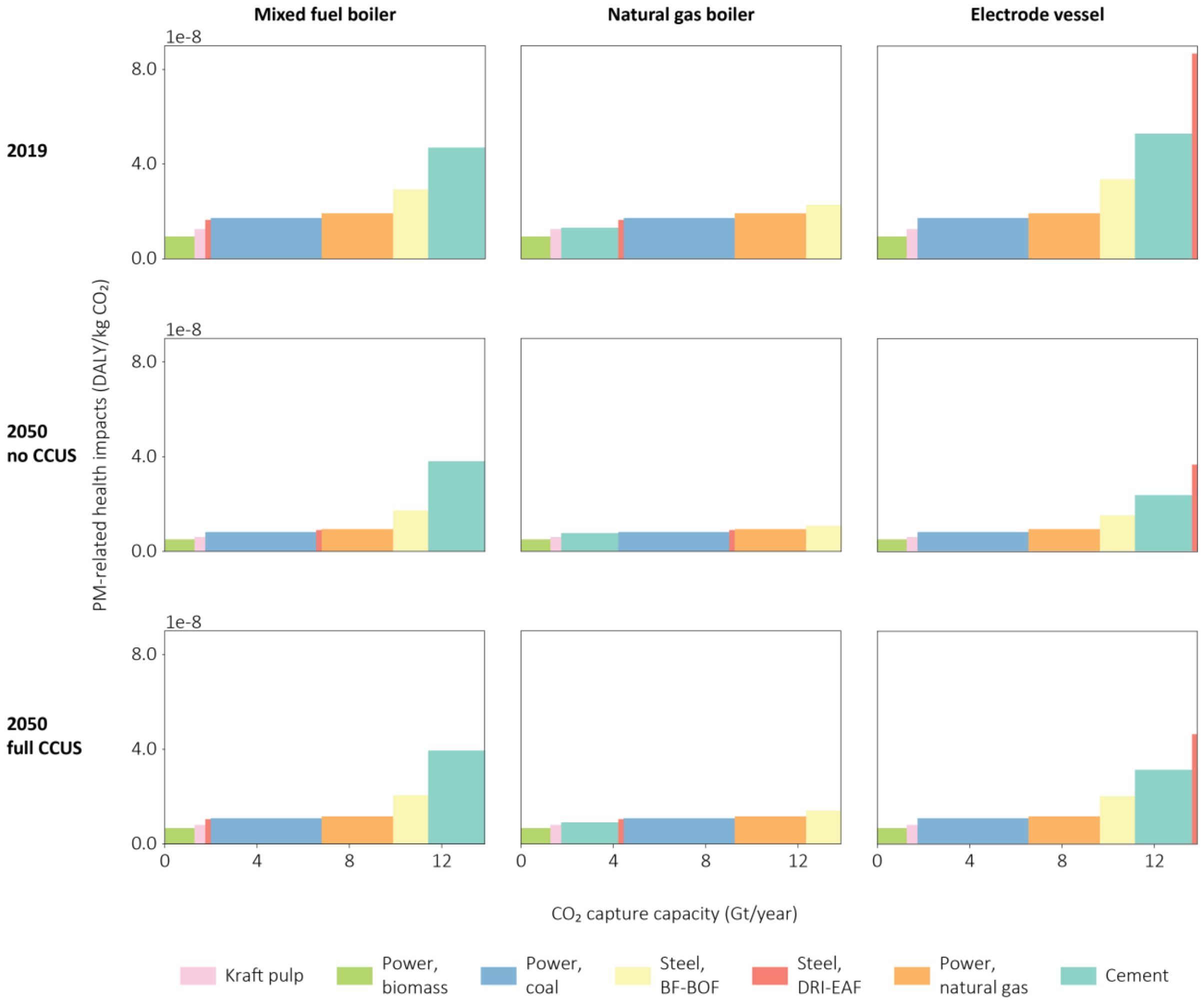


Fig. S4 Environmental-merit-order curve for PM-related health impacts of 1 kg CO_2 captured from different industries under the high-emission scenario with different combinations of electricity and steam sources

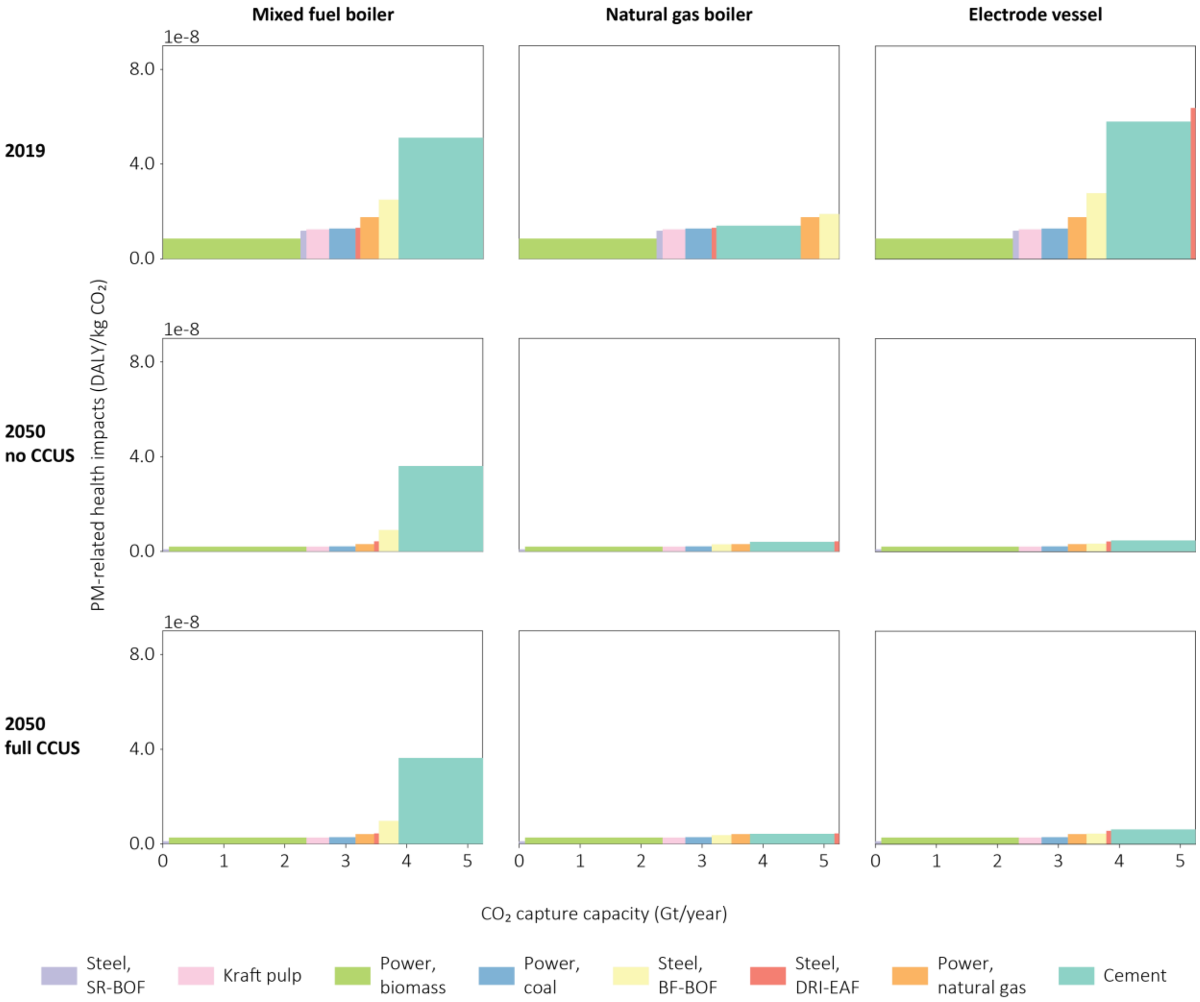


Fig. S5 Environmental-merit-order curve for PM-related health impacts of 1 kg CO_2 captured from different industries under the low-emission scenario with different combinations of electricity and steam sources

S2.2 Bottom-up case studies: optimization of CO_2 supply to chemical manufacturing sites in China

S2.2.1 Basic scenario

Table S53 Optimization results from the basic scenario

Item	Unit	When minimizing total climate change impacts	When minimizing total health impacts
Total transportation distance:	km	64146	53385
Average transportation distance to each chemical manufacturing site:	km	224	182
Total climate change impacts from carbon capture:	kt CO_2-eq	206101	218153
Total climate change impacts from transportation:	kt CO_2-eq	21278	17243
Total climate change impacts	kt CO_2-eq	227379	235395
Total health impacts from carbon capture:	DALY	4819	5115
Total health impacts from transportation:	DALY	3006	2436
Total health impacts	DALY	7824	7550

S2.2.2 Sensitivity analysis 1: CO_2 transportation with pipelines

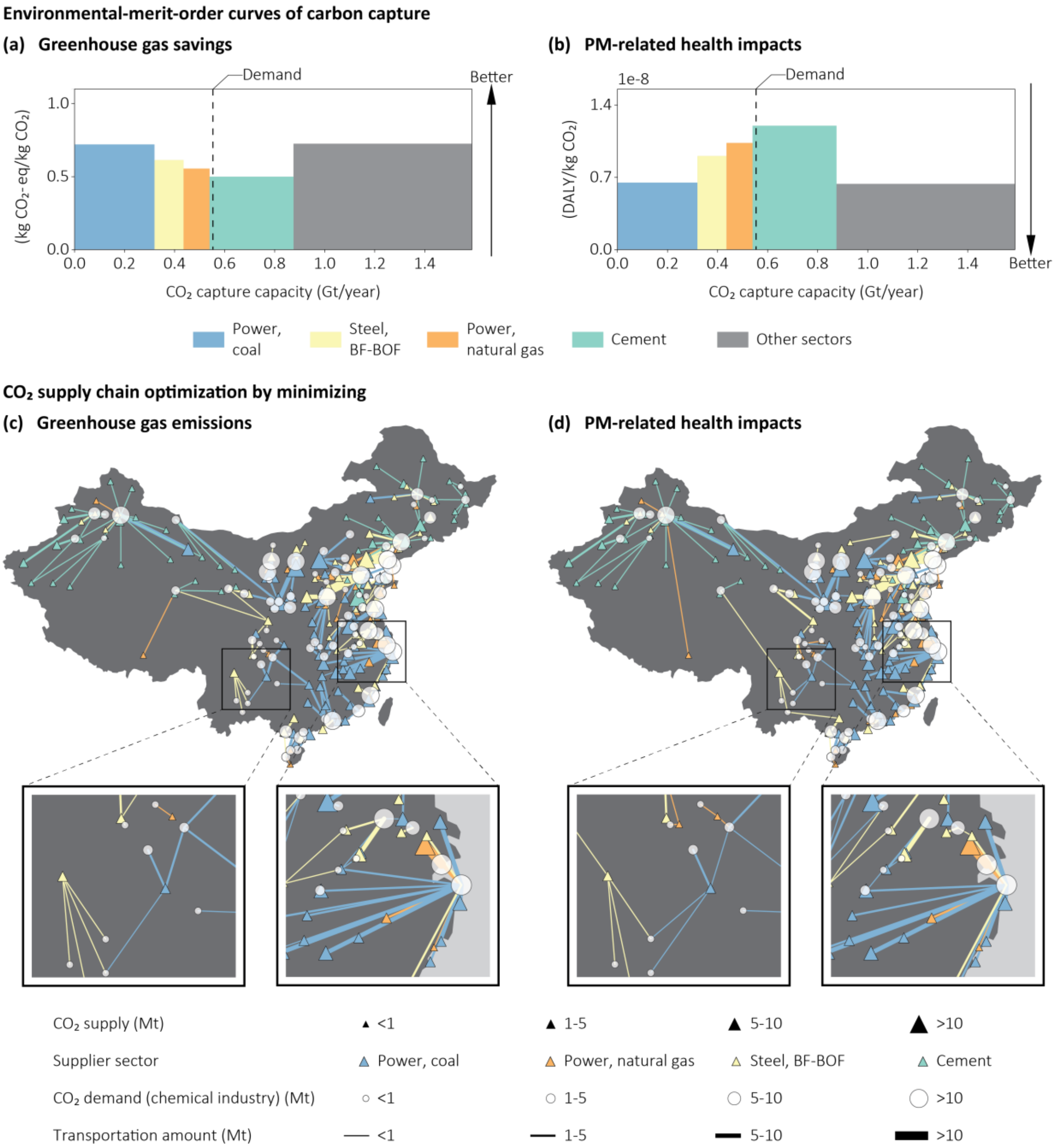


Fig. S6 (a) and (b): GHG savings and PM-related health impacts of carbon capture from different sectors in China. (c) and (d): CO_2 supply chain optimization in China under the low-emission scenario in 2050 with pipeline transportation by minimizing the total regional GHG emissions and the total regional PM-related health impacts.

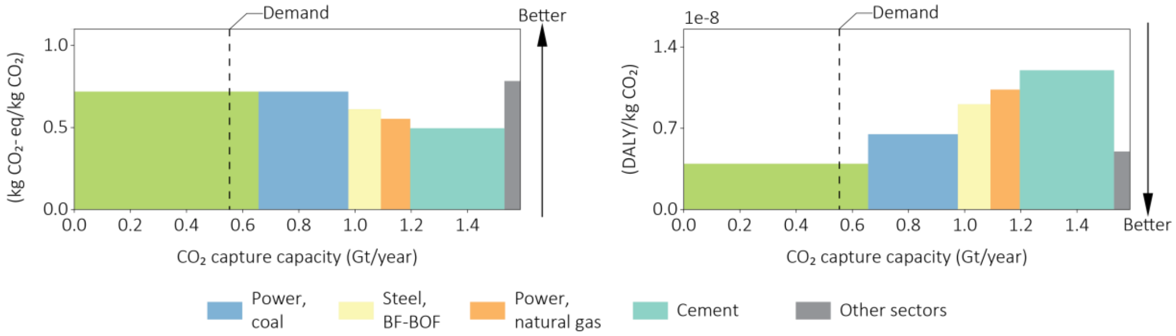
Table S54 Optimization results from sensitivity analysis 1: CO_2 transportation with pipelines

Item	Unit	When minimizing total climate change impacts	When minimizing total health impacts
Total transportation distance:	km	68971	73150
Average transportation distance to each chemical manufacturing site:	km	227	233
Total climate change impacts from carbon capture:	kt CO_2-eq	205934	205759
Total climate change impacts from transportation:	kt CO_2-eq	8917	9163
Total climate change impacts	kt CO_2-eq	214851	214922
Total health impacts from carbon capture:	DALY	4812	4805
Total health impacts from transportation:	DALY	193	198
Total health impacts	DALY	5005	5003

S2.2.3 Sensitivity analysis 2: solid biomass-fired power plants included as potential CO_2 suppliers

Environmental-merit-order curves of carbon capture

(a) Greenhouse gas savings **(b) PM-related health impacts**



CO_2 supply chain optimization by minimizing

(c) Greenhouse gas emissions **(d) PM-related health impacts**

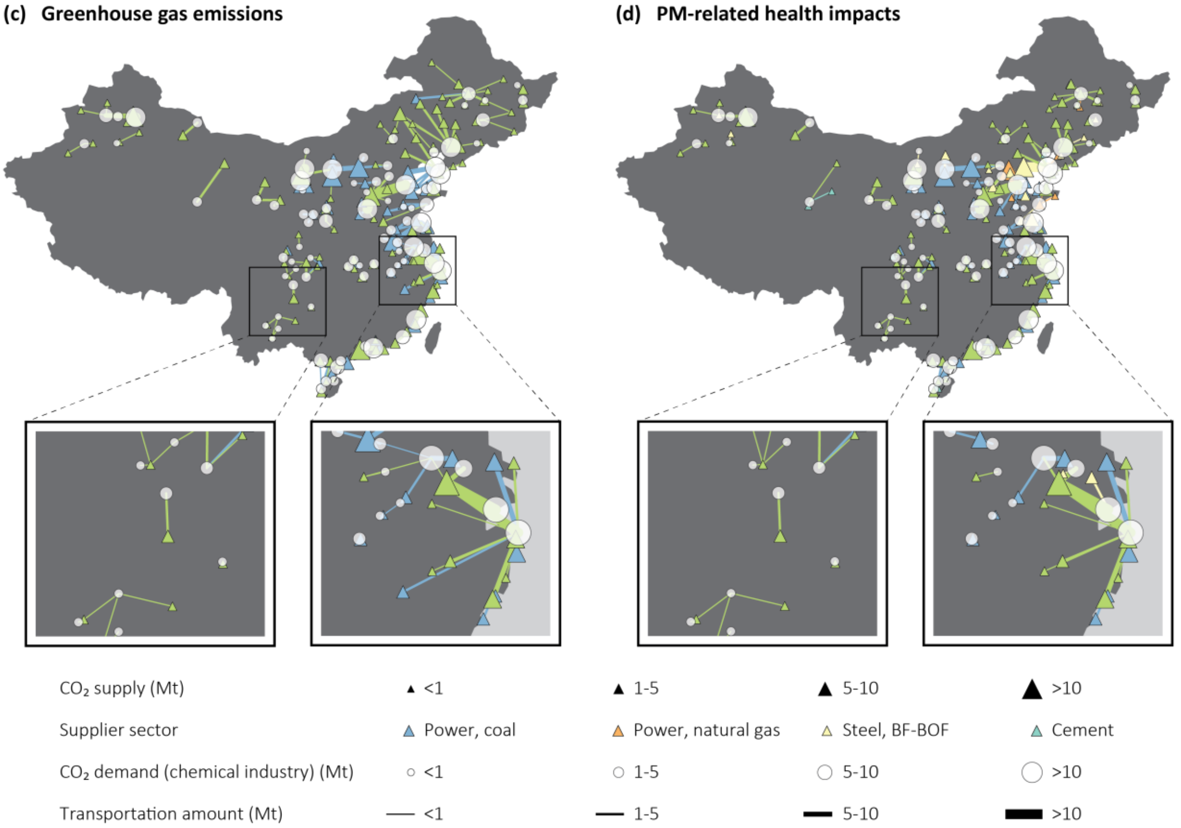


Fig. S7 (a) and (b): GHG savings and PM-related health impacts of carbon capture from different sectors in China. (c) and (d): CO_2 supply chain optimization in China under the low-emission scenario in 2050 with truck transportation and with biomass-fired power plants as potential suppliers by minimizing the total regional GHG emissions and the total regional PM-related health impacts.

Table S55 Optimization results from sensitivity analysis 2: solid biomass-fired power plants included as potential CO_2 suppliers

Item	Unit	When minimizing total climate change impacts	When minimizing total health impacts
Total transportation distance:	km	30063	25026
Average transportation distance to each chemical manufacturing site:	km	170	131
Total climate change impacts from carbon capture:	kt CO_2-eq	170437	181267
Total climate change impacts from transportation:	kt CO_2-eq	16188	12462
Total climate change impacts	kt CO_2-eq	186625	193729
Total health impacts from carbon capture:	DALY	3954	4214
Total health impacts from transportation:	DALY	2287	1760
Total health impacts	DALY	6240	5975

References

1. IEA, *Technology roadmap: low-carbon transition in the cement industry*, International Energy Agency, Paris, France, 2018.
2. IEA, *Iron and steel technology roadmap: towards more sustainable steelmaking*, International Energy Agency, Paris, France, 2020.
3. IEA, *World energy outlook 2020*, International Energy Agency, Paris, France, 2020.
4. IEA, *World energy outlook 2021*, International Energy Agency, Paris, France, 2021.
5. IEA, *Net zero by 2050: A roadmap for the global energy sector*, International Energy Agency, Paris, France, 2021.
6. H. Kim, H. McJeon, D. Jung, H. Lee, C. Bergero and J. Eom, *[Under review]*, 2022.
7. IEA, *World energy statistics and balances*, International Energy Agency, 2021.
8. T. Lecomte, J. Félix Ferrería de la Fuente, F. Neuwahl, M. Canova, A. Pinasseau, I. Jankov, T. Brinkmann, S. Roudier and L. Delgado Sancho, *Best Available Techniques (BAT) reference document for large combustion plants*, the Joint Research Centre of the European Commission (JRC), Luxembourg, Luxembourg, 2017.
9. IPCC, *IPCC special report on carbon capture and storage*, International Panel on Climate Change, Cambridge, United Kingdom and New York, NY, USA, 2005.
10. IPCC, *IPCC guidelines for national greenhouse gas inventories*, International Panel on Climate Change, Hayama, Japan, 2006.
11. World Steel Association, *Steel statistical yearbook 2020*, Brussels, Belgium, 2020.
12. P. Wang, M. Ryberg, Y. Yang, K. S. Feng, S. Kara, M. Hauschild and W. Q. Chen, *Nat. Commun.*, 2021, **12**.
13. Material Economics, *Industrial transformation 2050: Pathways to net-zero emissions from EU heavy industry*, Stockholm, Sweden, 2019.
14. A. Hasanbeigi and C. Springer, *How clean is the U.S. steel industry? An international benchmarking of energy and CO_2 intensities*, Global Efficiency Intelligence, San Francisco, CA, USA, 2019.
15. N. A. Ryan, S. A. Miller, S. J. Skerlos and D. R. Cooper, *Environ. Sci. Technol.*, 2020, **54**, 14598-14608.
16. USGS, *Mineral commodity summaries 2021*, U.S. Geological Survey, Reston, VA, 2021.
17. Korea Cement Association (KCA), Monthly production, http://www.cement.or.kr/english/stati/mm_pro_view.asp, (accessed October, 2021).
18. The European Cement Association (CEMBUREAU), Key facts & figures, https://cembureau.eu/about-our-industry/key-facts-figures/, (accessed October, 2021).
19. Energy Transition Commission, *China 2050: a fully developed rich zero-carbon economy*, Beijing, China, 2019.
20. J. H. Xu, T. Fleiter, Y. Fan and W. Eichhammer, *Appl. Energy*, 2014, **130**, 592-602.
21. F. Schorcht, I. Kourti, B. M. Scalet, S. Roudier and L. D. Sancho, *Best available techniques (BAT) reference document for the production of cement, lime and magnesium oxide*, the Joint Research Centre of the European Commission (JRC), Luxembourg, Luxembourg, 2013.
22. T. P. Hills, M. G. Sceats and P. S. Fennell, in *Rsc Energy Environ S*, eds. M. Bui and N. M. Dowell, The Royal Society of Chemistry, Croydon, UK, 2020, DOI: 10.1039/9781788012744, ch. 10, pp. 315-352.

23. Food and Agriculture Organization of the United Nations (FAO), Forestry production and trade, http://www.fao.org/faostat/en/#data/FO/, (accessed October, 2021).
24. J. Buongiorno, *Sustainability-Basel*, 2021, **13**.
25. International Energy Agency (IEA), Pulp and Paper, https://www.iea.org/reports/pulp-and-paper, (accessed March, 2022).
26. IEAGHG, *Techno-economic evaluation of retrofitting CCS in a market pulp and integrated pulp and board mill*, IEA Greenhouse Gas R&D Programme, Cheltenham, UK, 2016.
27. U.S. Department of Energy, *Bandwidth study on energy use and potential energy saving opportunities in U.S. pulp and paper manufacturing*, 2015.
28. China Nitrogen Fertilizer Industry Association (CNFIA), Nitrogen fertilizer production and operation report in 2019 (in Chinese), http://www.cnfia.com.cn/c/cn/news/2020-05/08/news_12258.html, (accessed February, 2022).
29. International Fertilizer Association (IFA), Urea stats 2008-2019, https://www.ifastat.org/supply/Nitrogen%20Products/Urea, (accessed October, 2021).
30. Food and Agriculture Organization of the United Nations (FAO), Fertilizers by product, https://www.fao.org/faostat/en/#data/RFB, (accessed October, 2021).
31. USGS, Nitrogen statistics and information, https://www.usgs.gov/centers/nmic/nitrogen-statistics-and-information, (accessed October, 2021).
32. M. Chakravarty, *How will methanol survive the oversupply?*, Argus Media group, Taipei, 2019.
33. Methanol Institute, Methanol price and supply/demand, https://www.methanol.org/methanol-price-supply-demand/, (accessed February, 2022).
34. Ministry of Chemicals and Fertilizers of India, *Chemicals and petrochemicals statistics at a glance – 2019*, New Delhi, India, 2020.
35. statista, Methanol production in the United States from 1990 to 2019, https://www.statista.com/statistics/974802/us-methanol-production-volume/, (accessed October, 2021).
36. the National Bureau of Statistics of the People’s Republic of China, Annual national statistics (in Chinese) (2021), https://data.stats.gov.cn/easyquery.htm?cn=C01, (accessed October, 2021).
37. Petrochemicals Europe, European market overview, https://www.petrochemistry.eu/about-petrochemistry/petrochemicals-facts-and-figures/european-market-overview/, (accessed October, 2021).
38. Chemicals & Petrochemicals Manufacturers’ Association of India, India demand supply, http://cpmaindia.com, (accessed October, 2021).
39. the Ministry of Economy, Trade and Industry of Japan, Yearbook of current production statistics: chemical industry, https://www.meti.go.jp/statistics/tyo/seidou/result/ichiran/resourceData/02_kagaku/nenpo/h2dbb2020k.xls, (accessed October, 2021).
40. Statistics Korea, Volume of production, shipment, inventory, domestic demand and exports,

https://kosis.kr/statHtml/statHtml.do?orgId=101&tblId=DT_1F01512&conn_path=I2&language=en, (accessed October, 2021).
41. ESI Africa, Global ethylene capacity to see considerable growth of 27%, https://www.esi-africa.com/industry-sectors/business-and-markets/global-ethylene-capacity-to-see-considerable-growth-of-27/, (accessed October, 2021).
42. IHS Markit, Petrochemical capacity in China and Middle East: Growth amid challenges, https://ihsmarkit.com/research-analysis/petrochemical-capacity-growth-in-china-middle-east.html, (accessed October, 2021).
43. GPCA, *GPCA annual report 2020: Transitioning into the new reality*, Gulf Petrochemicals and Chemicals Association, Dubai, United Arab Emirates, 2020.
44. Eurasian Chemical Market International Magazine, Production and market of ethylene in Russia and the CIS countries, http://www.chemmarket.info/en/home/article/3286/. (accessed October, 2021).
45. statista, Production of selected chemicals and plastics in the United States in 2019, by type, https://www.statista.com/statistics/299725/total-us-plastics-and-chemicals-shipments-by-type/, (accessed October, 2021).
46. statista, Ethylene demand and production capacity worldwide from 2015 to 2022, https://www.statista.com/statistics/1246694/ethylene-demand-capacity-forecast-worldwide/, (accessed October, 2021).
47. CHYXX, Chinese propylene market and the operation of key companies in 2019 (in Chinese), https://www.chyxx.com/industry/202008/888750.html, (accessed October, 2021).
48. INDEXBOX, Propylene market, https://app.indexbox.io/report/290122/, (accessed October, 2021).
49. Deloitte, *The future of petrochemicals: growth surrounded by uncertainty*, 2019.
50. statista, Propylene demand and production capacity worldwide from 2015 to 2022, https://www.statista.com/statistics/1246689/propylene-demand-capacity-forecast-worldwide/, (accessed October, 2021).
51. CPCIF, *CPCIF annual report 2019*, China Petroleum and Chemical Industry Federation, Beijing, China, 2019.
52. huaon, The production, demand, and import analysis of para-xylene in China in 2019 (in Chinese), https://www.huaon.com/channel/trend/670361.html, (accessed October, 2021).
53. P. G. Levi and J. M. Cullen, *Environ Sci Technol*, 2018, **52**, 1725-1734.
54. Aromatics Online, Facts and figures, https://www.aromaticsonline.eu/aromatics/facts-and-figures, (accessed October, 2021).
55. IEA, *The future of petrochemicals*, International Energy Agency, Paris, France, 2018.
56. W. Hall, T. Spencer, G. Renjith and S. Dayal, *The Potential Role of Hydrogen in India: A pathway for scaling-up low carbon hydrogen across the economy*, The Energy and Resources Institute (TERI), New Delhi, India, 2020.
57. X. Zhang, E. A. Davidson, D. L. Mauzerall, T. D. Searchinger, P. Dumas and Y. Shen, *Nature*, 2015, **528**, 51-59.
58. D. Saygin and D. Gielen, *Energies*, 2021, **14**.
59. A. M. Bazzanella and F. Ausfelder, *Low carbon energy and feedstock for the European chemical industry*, DECHEMA, Frankfurt am Main, Germany, 2017.

60. L. Y. Zhang, Q. Shen, M. Q. Wang, N. N. Sun, W. Wei, Y. Lei and Y. J. Wang, *J. Clean. Prod.*, 2019, **210**, 1131-1140.
61. International CCS Knowledge Centre, *The Shand CCS feasibility study (public report)*, Regina, SK, Canada, 2018.
62. IEAGHG, *Towards zero emissions: CCS in power plants using higher capture rates or biomass*, IEA Greenhouse Gas R&D Programme, Cheltenham, UK, 2019.
63. IEAGHG, *Iron and steel CCS study (techno-economics integrated steel mill)*, IEA Greenhouse Gas R&D Programme, Cheltenham, UK, 2013.
64. K. Volkart, C. Bauer and C. Boulet, *Int. J. Greenh. Gas Control*, 2013, **16**, 91-106.
65. Lockwood Greene, *Ironmaking process alternatives screening study*, U.S. Department of Energy, 2000.
66. Tata Steel, *HIsarna: building a sustainable steel industry*, 2020.
67. IFC, *Waste heat recovery for the cement sector: market and supplier analysis*, International Finance Corporation, 2014.
68. G. Wernet, C. Bauer, B. Steubing, J. Reinhard, E. Moreno-Ruiz and B. Weidema, *Int J Life Cycle Ass*, 2016, **21**, 1218-1230.
69. ecoinvent, *ecoinvent 3.8 dataset documentation*, 2021.
70. ecoinvent, Electricity - ecoinvent, https://ecoinvent.org/the-ecoinvent-database/sectors/electricity/, (accessed February, 2022).
71. C. Mutel, *Journal of Open Source Software*, 2017, **2**, 236.
72. L. Vandepaer and T. Gibon, *Int J Life Cycle Ass*, 2018, **23**, 970-977.
73. BSI, *PAS 2050: Specification for the assessment of the life cycle greenhouse gas emissions of goods and services*, British Standards Institution, London, UK, 2011.
74. Forest Research, Typical calorific values of fuels, https://www.forestresearch.gov.uk/tools-and-resources/fthr/biomass-energy-resources/reference-biomass/facts-figures/typical-calorific-values-of-fuels/, (accessed February, 2022).
75. F. Pittau, F. Krause, G. Lumia and G. Habert, *Build. Environ.*, 2018, **129**, 117-129.
76. F. Cherubini, G. P. Peters, T. Berntsen, A. H. Stromman and E. Hertwich, *Glob. Change Biol. Bioenergy*, 2011, **3**, 413-426.
77. C. Oberschelp, S. Pfister and S. Hellweg, unpublished work.
78. U.S. EPA, *Draft revisions to AP-42 Chapter 1, Section 6 - wood residue combustion in boilers* U.S. Environmental Protection Agency, NC, United States, 2021.
79. C. Oberschelp, S. Pfister and S. Hellweg, *Environ. Sci. Technol.*, 2020, **54**, 16028-16038.
80. Forschungsstelle für Energiewirtschaft e.V., *Kurzstudie Power-to-X. Ermittlung des Potenzials von PtX-Anwendungen für die Netzplanung der deutschen ÜNB (in German)*, Munich, Germany, 2017.
81. Global Energy Monitor, Global Steel Plant Tracker, https://globalenergymonitor.org/projects/global-steel-plant-tracker/, (accessed January, 2022).
82. Global Energy Monitor, Global Coal Plant Tracker, https://globalenergymonitor.org/projects/global-coal-plant-tracker/, (accessed January, 2022).

83. Global Energy Monitor, Global Gas Plant Tracker, https://globalenergymonitor.org/projects/global-gas-plant-tracker/, (accessed January, 2022).
84. R. Y. Cui, N. Hultman, D. Cui, H. McJeon, S. Yu, M. R. Edwards, A. Sen, K. Song, C. Bowman, L. Clarke, J. Kang, J. Lou, F. Yang, J. Yuan, W. Zhang and M. Zhu, *Nat. Commun.*, 2021, **12**, 1468.
85. C. Wildbolz, Diploma Thesis, ETH Zurich, 2007.