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## Net-zero transition of the global chemical industry with CO<sub>2</sub>-feedstock by 2050: feasible yet challenging†

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Carbon capture, utilization and storage (CCUS) have been projected by the power and industrial sectors to play a vital role towards net-zero greenhouse gas emissions. In this study, we aim to explore the feasibility of a global chemical industry that fully relies on CO<sub>2</sub> as its carbon source in 2050. We project the global annual CO<sub>2</sub> demand as chemical feedstock to be 2.2–3.1 gigatonnes (Gt), well within the possible range of supply (5.2–13.9 Gt) from the power, cement, steel, and kraft pulp sectors. Hence, feedstock availability is not a constraint factor for the transition towards a fully CO<sub>2</sub>-based chemical industry on the global basis, with the exception of few regions that could face local supply shortages, such as the Middle East. We further conduct life cycle assessment to examine the environmental benefits on climate change and the trade-offs of particulate matter-related health impacts induced by carbon capture. We conclude that CO<sub>2</sub> captured from solid biomass-fired power plants and kraft pulp mills in Europe would have the least environmental and health impacts, and that India and China should prioritize low-impact regional electricity supply before a large-scale deployment of CCUS. Finally, two bottom-up case studies of China and the Middle East illustrate how the total regional environmental and health impacts from carbon capture can be minimized by optimizing its supply sources and transport, requiring cross-sectoral cooperation and early planning of infrastructure. Overall, capture and utilization of unabatable industrial waste CO<sub>2</sub> as chemical feedstock can be a feasible way for the net-zero transition of the industry, while concerted efforts are yet needed to build up the carbon-capture-and-utilization value chain around the world.

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## 1. Introduction

While the chemical industry is an enabler for achieving the Sustainable Development Goals,<sup>1,2</sup> it is also the third-largest greenhouse gas (GHG) emitting sector and the largest consumer of fossil fuels among industrial sectors.<sup>3</sup> In 2019, in addition to 19.5 exajoule (EJ) of process energy consumption, the chemical industry was also responsible for 27.9 EJ of energy consumption in the form of feedstocks.<sup>4</sup> Thus, switching to renewable process energy alone is not sufficient to reach net-zero GHG emissions of the chemical industry. Replacing

fossil feedstocks with renewable or recycled ones is also essential for further minimizing the industry's GHG emissions and for its transition towards a circular economy.<sup>5</sup>

In recent years, carbon dioxide (CO<sub>2</sub>)—the major GHG—has been proposed as a candidate feedstock that may enable the aforementioned transition of the chemical industry. In particular, various carbon-utilization technologies have been and are being developed to produce commodity chemicals from CO<sub>2</sub>, including through reduction and carboxylation reactions.<sup>6,7</sup> A detailed analysis of potential CO<sub>2</sub>-based synthesis routes towards bulk and fine chemicals can be found in the work by Otto *et al.*<sup>8</sup> Recent studies have increasingly focused on developing novel and cost-effective catalysts that enable high selectivity and conversion rates of desired products under mild reaction conditions.<sup>6,9–14</sup> In 2020, China launched a demonstration project that aims to produce 1000 tonnes of CO<sub>2</sub>-derived methanol annually.<sup>15</sup> As such, CO<sub>2</sub> utilization as a renewable feedstock seemingly creates an ideal win-win situation that simultaneously combats global warming and enables a more sustainable chemical industry. However, to understand the feasibility of the concept, factors

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such as the regional supply security of CO<sub>2</sub> need to be assessed against current and foreseeable mega-trends, which may sometimes work in an antagonistic manner.

34 gigatonnes (Gt) of CO<sub>2</sub> were emitted globally from fossil fuels in 2019, 60% of which came from point sources of the power generation and industrial sectors where many emissions are hard to abate.<sup>16</sup> Carbon capture has been projected to play a vital role in tackling these large-scale point emissions in most of the pathways towards limiting the temperature increase within 1.5 °C underlined by the Intergovernmental Panel on Climate Change (IPCC).<sup>17</sup> It has also been adopted as part of the long-term low emissions and development strategies by 83% of the national submissions under the Paris agreement.<sup>18</sup> Therefore, while the global capacity of carbon capture in operation is less than 40 megatonnes (Mt) by the end of 2021,<sup>18</sup> an accelerated deployment of carbon-capture projects may be expected, resulting in increases in CO<sub>2</sub> supply for industrial use.

Meanwhile, to avoid catastrophic consequences of global warming, industrial sectors are developing roadmaps towards net-zero GHG emissions by 2050, including using renewable energy sources, improving efficiency, and switching to innovative low-carbon production routes.<sup>19–23</sup> These trends imply that overall industrial CO<sub>2</sub> emissions may drastically decrease in the future, resulting in reduced CO<sub>2</sub> availability for carbon capture. In addition, there are other mechanisms for captured CO<sub>2</sub>, *e.g.*, direct storage in geological reservoirs (known as carbon capture and storage, or CCS),<sup>24</sup> and production of synthetic fuels.<sup>25,26</sup> Each mechanism has its own advantages and disadvantages. For example, CCS could contribute to the long-term removal of CO<sub>2</sub> from the atmosphere,<sup>27</sup> but the regional storage capacity might remain a challenge, especially in India and China.<sup>28</sup> Public concerns, including safety considerations, are another obstacle yet to be addressed.<sup>29</sup> The deployment of these mechanisms could determine the local supply of captured CO<sub>2</sub> for the chemical industry. To our knowledge, no detailed studies have addressed the future dynamics of regional CO<sub>2</sub> supply-demand balance.

Furthermore, CO<sub>2</sub> capture is not free from environmental impacts. Chemical absorption with monoethanolamine (MEA), the currently most mature carbon-capture technology, is known for its high energy penalty, especially due to reboiler duty for solvent regeneration.<sup>24,30</sup> Life cycle assessment (LCA) is a key method for evaluating the environmental benefits and trade-offs of carbon capture. Several LCA studies have been conducted for carbon capture in individual regions (*e.g.*, Europe) and sectors (*e.g.*, coal-fired power plants).<sup>31–33</sup> However, the environmental impacts of carbon capture depend on the regions and sectors from which CO<sub>2</sub> is captured, as well as electricity and fuel mixes used to perform carbon capture, highlighting the need for cross-regional and cross-sectoral assessments. Von der Assen *et al.*<sup>34</sup> have benchmarked the environmental impacts of carbon capture from different industrial sectors in Europe using LCA, including global warming impacts and fossil resources depletion. They concluded that CO<sub>2</sub> should first be captured from the sites

where CO<sub>2</sub> concentration in the flue gas is close to 100%, followed by paper mills and coal power plants. A follow-up study further pointed out that GHG savings can be significantly improved if the carbon-capture process uses renewable energy instead of the current electricity grid mix in Europe.<sup>35</sup> However, both studies did not consider future global dynamics of the CO<sub>2</sub> supply-demand relationships, regions outside Europe, and other impacts such as particulate matter (PM)-related health impacts, which are largely driven by fossil-energy use.<sup>36,37</sup>

Against these knowledge gaps, we endeavor in this study to provide insights into the strategic planning of future sustainable transitions of the global chemical industry, with a particular focus on exploring the supply-demand feasibility of a chemical industry in 2050 that fully relies on CO<sub>2</sub> as its carbon source. We acknowledge that other potential net-zero transition pathways also exist for the chemical industry, *e.g.*, through biomass valorization; these pathways will be assessed in our subsequent studies. Here, we start with the assessment of the future global and regional supply-demand balance of CO<sub>2</sub>, and then use LCA to examine the regional and sectoral savings on climate change impacts and trade-offs of PM-related health impacts for capturing 1 kilogram (kg) of CO<sub>2</sub>. Based on the LCA results, we explore a regionalized sourcing strategy of CO<sub>2</sub>-feedstock, which is demonstrated by two bottom-up case studies, China and the Middle East. We further discuss our findings and their implications for future research and climate mitigation measures.

## 2. Methods

The study consists of three parts (see Fig. 1): (I) regional CO<sub>2</sub> supply-demand balance in 2050, (II) regionalized environmental and health impacts of CO<sub>2</sub> capture from different sectors, and (III) case studies of regionalized CO<sub>2</sub> sourcing strategies.

### 2.1 Global and regional supply-demand balance of CO<sub>2</sub>

The potential regional CO<sub>2</sub> supply from the power and industrial sectors, and its demand as chemical feedstock in 2050 were projected under two CO<sub>2</sub>-emission scenarios that were intended to cover the possible range of uncertainties.<sup>38</sup> The high-emission scenario was set according to the conservative scenarios defined by the International Energy Agency (IEA), such as the Stated Policies Scenario. The low-emission scenario was assumed to be the ambitious scenario that is compatible with IEA's Net Zero Emissions by 2050 Scenario, or equivalent. The detailed scenario settings of each sector are described in sections S1.1 and S1.2 in ESI.†

The following nine countries/regions of focus were chosen as they are the world's current largest CO<sub>2</sub> emitters, the largest primary chemical producers, and/or under rapid development: China (CN), the United States of America (US), India (IN), the European Union (EU), Japan (JP), the Republic of Korea (KR), the Russian Federation (RU), Region Middle East (RME), and



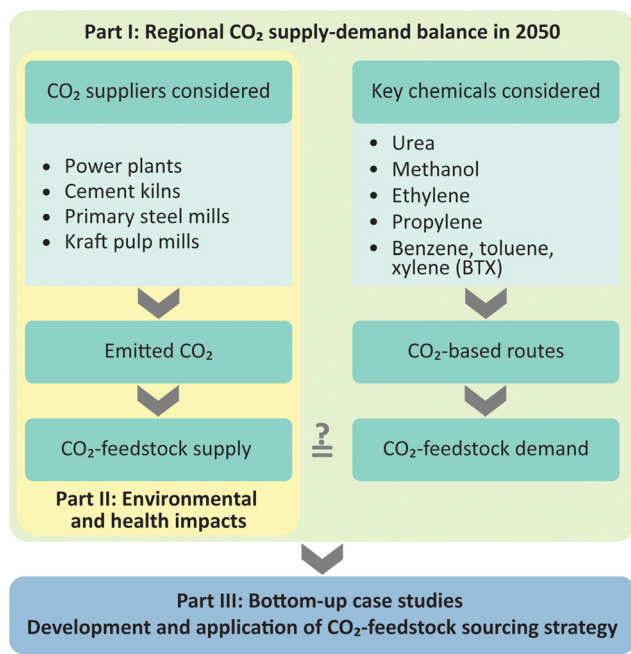


Fig. 1 Study overview.

Region Africa (RAF) (see Table S2 in ESI† for the region definitions). In 2019, these regions together account for 75% of the global CO<sub>2</sub> emissions<sup>16</sup> and 90% of the global production of the seven base chemicals that are the current key building blocks for the bulk of the chemical industry (Table S7 in ESI†): ammonia, methanol, ethylene, propylene, and benzene, toluene and xylenes (BTX aromatics).<sup>3</sup> All other countries were grouped together as “Rest of the World” (RoW).

**2.1.1 Estimating CO<sub>2</sub> supply from the power and industrial sectors.** For CO<sub>2</sub> supply, the power, steel, and cement sectors were selected, as they are the current largest fossil CO<sub>2</sub> emission sources.<sup>39</sup> Moreover, the kraft pulp sector was included, which is the largest biogenic CO<sub>2</sub> source according to a Europe-focused study.<sup>40</sup> In particular, large stationary sources that emit more than 0.1 Mt CO<sub>2</sub> per year were considered. These include power plants (coal, natural gas, and solid biomass-fueled), cement kilns, primary steel mills, and kraft pulp mills. The primary steel mills include the blast furnace-basic oxygen furnace (BF-BOF) route, the direct reduced iron-electric arc furnace (DRI-EAF) route, and the smelting reduction-basic oxygen furnace (SR-BOF) route that is to be commercialized under the low-emission scenario in 2050.<sup>21</sup>

The sectoral CO<sub>2</sub> emissions were quantified by multiplying its projected product or energy output with the regionalized specific carbon emission intensity (which was determined by the production routes, type of fuels used, and energy efficiency). The production routes and type of fuels used are sector- and region-specific, with detailed descriptions in section S1.1 in ESI.† For energy efficiency, a global average of 30% improvement from industrial sectors was considered possible according to the United Nations Economic Commission for Europe.<sup>41</sup> For the high-emission scenario in

2050, we assumed that half of this energy-reduction potential would be realized, *i.e.*, 15% improvement in energy efficiency in comparison to the 2019 baseline, as long as the improvement does not exceed the best-available technology (BAT) level identified in the literature.<sup>22,42–44</sup> For the low-emission scenario, we assumed that all manufacturing facilities would be operating at the energy efficiency of their BAT level.

For CO<sub>2</sub> capture, a capturing rate of 90% from flue gas was assumed as the technical limit for both scenarios, as it is the common industrial practice.<sup>45–47</sup> For power plants, cement kilns, and kraft pulp mills, capturing CO<sub>2</sub> from all stacks was assumed; hence, the maximum CO<sub>2</sub> capture capacity from these sources would be 90% of the total emissions.

In integrated steel mills, due to land constraints and economic factors, it would be difficult to capture CO<sub>2</sub> from every stack. Thus, for BF-BOF steel mills, it was assumed that CO<sub>2</sub> would only be captured at four types of stacks with the largest CO<sub>2</sub> emission rates (the blast furnace hot stove, on-site steam generation plant, coke oven, and lime kiln), representing 72% of their total CO<sub>2</sub> emissions.<sup>47</sup> Combined with the 90% capture limit from flue gas, a maximum of 65% of the total CO<sub>2</sub> emissions could be captured. For other types of steel mills, capturing 80% of their total emissions was assumed.<sup>48</sup>

**2.1.2 Estimating CO<sub>2</sub>-feedstock demand from the chemical industry.** In terms of demand, a future CO<sub>2</sub>-based chemical industry was assumed to be still based on the seven base chemicals as key building blocks. These base chemicals were assumed to be the key CO<sub>2</sub> consumers, with the exception of ammonia. While ammonia does not contain carbon in its structure, urea—accounting for 55% of the downstream use of ammonia—is a direct CO<sub>2</sub> consumer.

The potential CO<sub>2</sub>-feedstock demand for a given chemical was calculated by multiplying the projected production volume of the chemical (in Mt per year) with the specific CO<sub>2</sub> demand in a given CO<sub>2</sub>-based production route (kg CO<sub>2</sub> per kg chemical). The production routes and their corresponding specific CO<sub>2</sub> demand were assumed to be the same in both high- and low-emission scenarios. The global and regional production volumes of the seven key chemicals in 2050 under the two scenarios were projected using the growth rates estimated by IEA (Tables S33 and S34 in ESI.†).<sup>3</sup> The CO<sub>2</sub>-based production routes considered either are already commercialized (urea, ethylene, and propylene), or have a high technology readiness level (TRL) (methanol and BTX aromatics).<sup>5,49</sup> The specific CO<sub>2</sub> demand was calculated through the stoichiometric balance of each production route, taking into account its corresponding conversion rate. Detailed descriptions of the CO<sub>2</sub>-based production routes for the seven key base chemicals can be found in section S1.2.2 in ESI.†

## 2.2 Environmental and health impacts of carbon capture

We assumed that 30 weight-% aqueous MEA would be applied to capture CO<sub>2</sub> from all the sectors, as it is currently the most mature technology with successful retrofitting applications in various industries.<sup>24</sup> The captured CO<sub>2</sub> was assumed to be compressed to 110 bar as a general industrial practice for



transportation.<sup>33</sup> The assessed impacts include climate change impacts, calculated with the global warming potential over 100 years (GWP100),<sup>50</sup> and PM-related health impacts.<sup>31,34</sup> The selection of these two impacts is because they are among the most relevant impacts for combustion of fossil fuels, the main source of environmental and health impacts with regard to carbon capture.

LCA was then performed to quantify the impacts of CO<sub>2</sub> capture from different sectors. The functional unit was defined as 1 kg of captured CO<sub>2</sub> compressed to 110 bar at the gate of carbon-capture facilities. Transportation was not considered in the global analysis, but its influence was evaluated in the detailed case studies below. Other utilization mechanisms of the captured CO<sub>2</sub> were excluded in this study, as the focus is on assessing the availability of CO<sub>2</sub> as feedstock and compare the impacts of different sources of CO<sub>2</sub> with each other.

The impacts of capturing 1 kg CO<sub>2</sub> were calculated as the difference of the impacts between each reference system (*e.g.*, power plants, cement kilns, steel mills, and kraft pulp mills) with and without carbon capture (the only changing variable). MEA make-up is around 1–2 gram per kg CO<sub>2</sub> captured, and according to the previous studies, its climate change and other environmental impacts are generally negligible compared to the energy use for carbon capture.<sup>31,33,51,52</sup> Therefore, the impacts of MEA were not estimated in this study.

Energy use plays an important role in determining the environmental and health impacts of carbon capture. Capturing 1 kg CO<sub>2</sub> typically requires 3.6–4.0 megajoule (MJ) of low-pressure steam for MEA regeneration,<sup>24</sup> in addition to around 0.17 kilowatt-hours (kW h) of electricity for pumping and CO<sub>2</sub> compression (Fig. S1 in ESI†).<sup>33</sup>

More specifically, in the power plants and kraft pulp mills, steam and electricity supply for carbon capture were assumed to be extracted directly from the power generation units within the system boundary, without additional external energy supply. However, as net energy exporters, their net electricity output would be less. Due to the complexity to identify marginal electricity suppliers acknowledged by the previous studies,<sup>34,53</sup> in this study, additional electricity from the regional electricity grid was assumed to be required to compensate for this power loss, contributing to the environmental and health impacts of carbon capture.

For cement kilns and steel mills, waste heat was assumed to be available for utilization by the carbon-capture process. Therefore, the steam for MEA regeneration was supplied with a waste-heat boiler wherever possible, prior to using the same additional fuel mix as for the main production process (*e.g.*, 100% coal in BF-BOF steel mills). As part of the sensitivity analysis, other scenarios were investigated where the steam was supplied with another natural gas boiler or using electrode vessels. The electricity needed for carbon capture was assumed to be supplied by the regional grid mix in 2019. Scenarios of the regional grid mix of electricity supply in 2050 based on IEA's World Energy Outlook<sup>54</sup> were also investigated as part of the sensitivity analysis. Detailed settings of the additional

energy requirement for carbon capture in different systems are provided in Table S37 in ESI.†

The “allocation, cut-off by classification” system model of ecoinvent 3.8 was used to calculate climate change impacts of regional electricity production from wind, hydro, geothermal, and nuclear power plants, as well as background processes of regional market fuel supply (coal, oil, natural gas, and biomass). Climate change and PM-related health impacts of per unit fuel combustion in the foreground processes of electricity and steam production were derived from the IPCC report<sup>50</sup> and Oberschelp *et al.*,<sup>36,39</sup> respectively. Detailed descriptions of the calculation of impact factors can be found in sections S1.3.2 and S1.3.3 in ESI,† while a discussion of the inherent uncertainties of the approach is provided by Oberschelp *et al.*<sup>36</sup>

### 2.3 Bottom-up case studies: development and application of CO<sub>2</sub>-feedstock sourcing strategies in China and the Middle East

China and the Middle East under the low-emission scenario in 2050 were selected as case studies to explore regionalized CO<sub>2</sub> sourcing strategies. They are the two largest producers of the base chemicals globally (Table S31 in ESI†). China is representative of regions with sufficient CO<sub>2</sub> supply to their chemical manufacturing sites, whereas the Middle East represents places with insufficient in-region supply of CO<sub>2</sub>-feedstock.

The geographical coordinates of existing large CO<sub>2</sub> point sources (*i.e.*, fossil-fueled power plants, cement kilns, and primary steel mills), and chemical manufacturing sites of the seven key chemicals and their respective production capacities were collected. Pulp mills (estimated to be less than 2% of the total CO<sub>2</sub> supply in both regions in 2050) were excluded from the case studies due to data gaps. SR-BOF steel mills and biomass-fired power plants were also excluded, as their locations in 2050 remain unknown, because these technologies were assumed to grow in the coming decades. However, as biomass-fired power plants would be a major CO<sub>2</sub> supplier in China in 2050, a scenario that considers solid biomass-fired power plants as CO<sub>2</sub> suppliers was investigated in the sensitivity analysis. To this end, to-be-eliminated coal-fired power plants, as described below, were assumed to be retrofitted into solid biomass-fired power plants to reduce stranded assets.<sup>55</sup>

The projected regional CO<sub>2</sub> demand by the chemical industry and supply by the different sectors were allocated to all the existing sites based on their current production capacities, except for the coal power plants in China and the gas power plants in the Middle East as many production capacities were expected to be eliminated under the low-emission scenario. Therefore, for these power plants, a simplified elimination strategy based on technical attributes including the age, size, technology, and application of the power generation units was adapted and applied according to Cui *et al.*<sup>56</sup> It was also assumed that no extra capacity of these power plants would be added other than the ones that have already been announced, permitted, or are under construction (see section S1.4.2 in ESI† for details).



Many chemical manufacturing sites are closely located in industrial parks. For a better map visualization, manufacturing sites within a 50-kilometer (km) circle were aggregated into chemical manufacturing clusters. The same aggregation was applied to each type of the CO<sub>2</sub> sources. The direct distance between each chemical manufacturing cluster and each CO<sub>2</sub> supply cluster within the region was calculated.

Transportation by trucks was assumed as a conservative assessment, as it represents the worst-case transportation scenario with the highest carbon footprint, and it does not require major infrastructure to be built. The dataset “transport, freight, lorry 16–32 metric ton, EURO3|RoW” in ecoinvent 3.8 was used to quantify the impacts of CO<sub>2</sub> transportation by trucks. Scenarios with pipeline transportation were investigated as a best-case transportation scenario in the sensitivity analysis (described in section S1.4.4 in ESI†).

Based on the environmental and health impacts of carbon capture and truck transportation (calculation details in section S1.4.3 in ESI†), a linear model was developed to optimize the supply amount from each CO<sub>2</sub> supply cluster *i* to each chemical manufacturing cluster *j* ( $x_{ij}$ ) that would minimize the total feedstock-related GHG emissions or PM-related health impacts (see eqn (1)):

$$\min \sum_i \sum_j (x_{ij} \text{DIST}_{ij} \text{IMPACT}_{ij}^{\text{TR}} + x_{ij} \text{IMPACT}_i^{\text{CC}}) \quad (1)$$

where  $\text{IMPACT}_{ij}^{\text{TR}}$  and  $\text{IMPACT}_i^{\text{CC}}$  represent the impact intensity (climate change impacts or PM-related health impacts) of transportation and carbon capture, respectively, and  $\text{DIST}_{ij}$  is the distance between *i* and *j*.

This objective function is subjected to the constraint of total CO<sub>2</sub> capture capacity of each supply cluster *i* ( $\text{TS}_i$ ) and the total CO<sub>2</sub> demand by each chemical manufacturing cluster *j* ( $\text{TD}_j$ ). If the regional supply would be able to cover its demand, the constraint functions are:

$$\begin{aligned} \sum_j x_{ij} &\leq \text{TS}_i \forall i \\ \sum_i x_{ij} &\geq \text{TD}_j \forall j \end{aligned} \quad (2)$$

where  $x_{ij}$  represents the CO<sub>2</sub> supply volume from supplier *i* to consumer *j*.

In the cases where regional supply would be insufficient to cover its demand and all regional supply would be used up, the constraints function become:

$$\begin{aligned} \sum_j x_{ij} &\geq \text{TS}_i \forall i \\ \sum_i x_{ij} &\leq \text{TD}_j \forall j \end{aligned} \quad (3)$$

## 3. Results

### 3.1 Global and regional supply-demand balance of CO<sub>2</sub>

The global mass flow of CO<sub>2</sub> in 2050 (Fig. 2a) indicates that the CO<sub>2</sub> demand from the chemical industry (2.2–3.1 Gt CO<sub>2</sub>-

feedstock) can be well covered by the global supply capacity: 6.6–16.6 Gt of fossil and biogenic CO<sub>2</sub> are projected to be emitted from the power plants, cement kilns, steel mills, and kraft pulp mills globally under the two scenarios, of which 5.6–14.0 Gt could be captured (around 85% of the emissions). In other words, the demand from the chemical industry makes up 22% and 42% of the maximum CO<sub>2</sub> capture capacity under high- and low-emission scenarios, respectively. The power sector is the largest CO<sub>2</sub> emitter under both scenarios. However, unlike the high-emission scenario, under which coal-fired power plants contribute to almost one-third of the total CO<sub>2</sub> emissions, biomass-fired power plants are potentially the major CO<sub>2</sub> supplier under the low-emission scenario.

Meanwhile, the CO<sub>2</sub> supply-demand balance has a very strong regional pattern (Fig. 2b). Among the nine countries/regions investigated in detail, China and India have the largest CO<sub>2</sub>-supply surplus under both the scenarios. In the EU, although fossil CO<sub>2</sub> emissions would decrease by almost 90% under the low-emission scenario in 2050 in comparison to 2019, biomass-fired power plants are projected to be rapidly deployed, emitting substantial amounts of biogenic CO<sub>2</sub>. As a result, it is estimated to have a large CO<sub>2</sub>-supply surplus of 0.45 Gt per year, next to China and India.

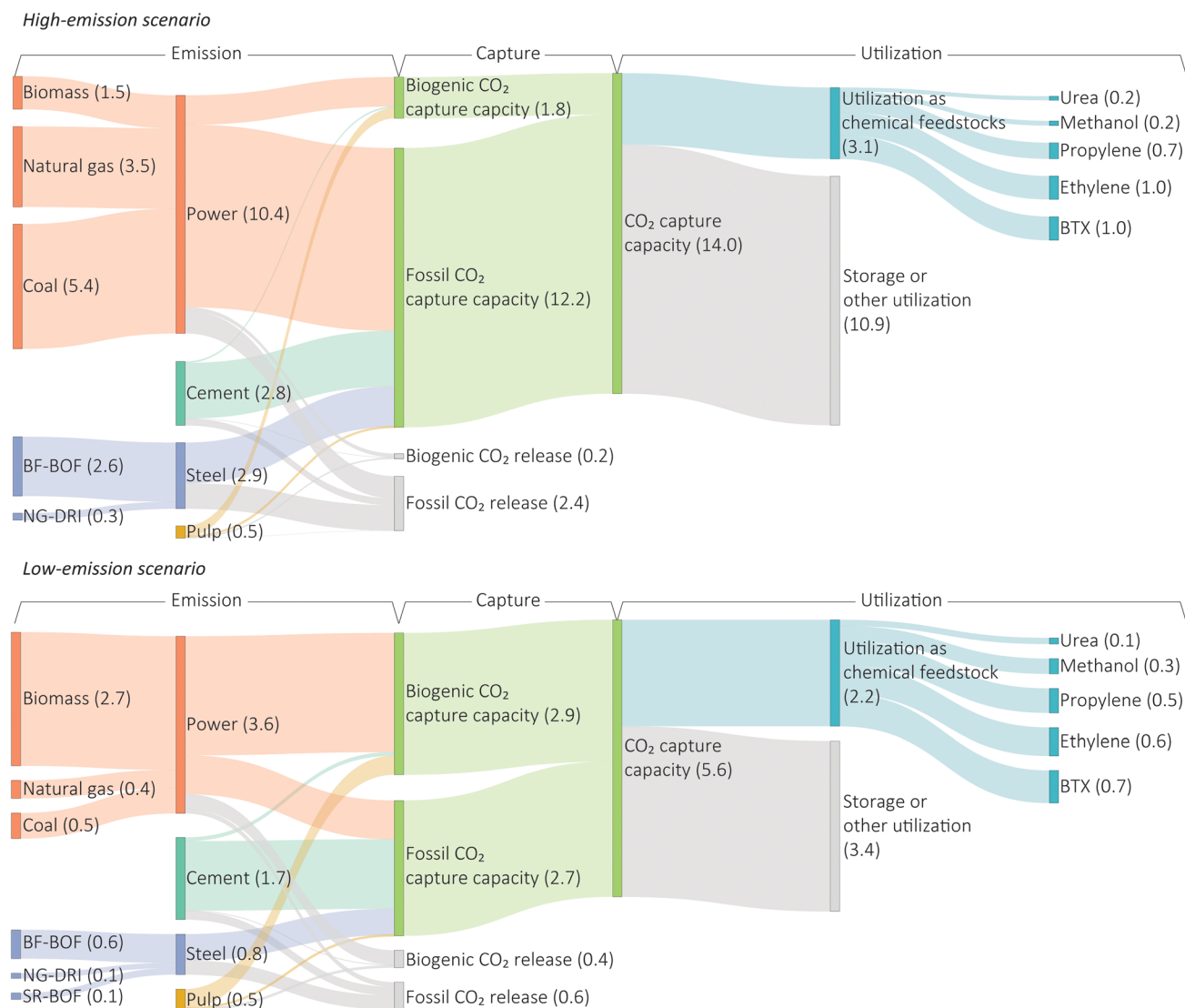
The Middle East region and the Republic of Korea, on the other hand, have relatively large chemical industries. However, CO<sub>2</sub> emissions under the low-emission scenario will drop drastically in comparison to 2019, mainly due to the decarbonization of the local electricity grid. Even if all CO<sub>2</sub>-feedstocks within the region were supplied, there would likely still be a supply shortage. The insufficient supply would especially be noteworthy for the chemical industry in the Middle East under the low-emission scenario, where only 27% of the CO<sub>2</sub> demand from the chemical industry could be fulfilled with its intra-regional supply.

### 3.2 Environmental and health impacts of carbon capture

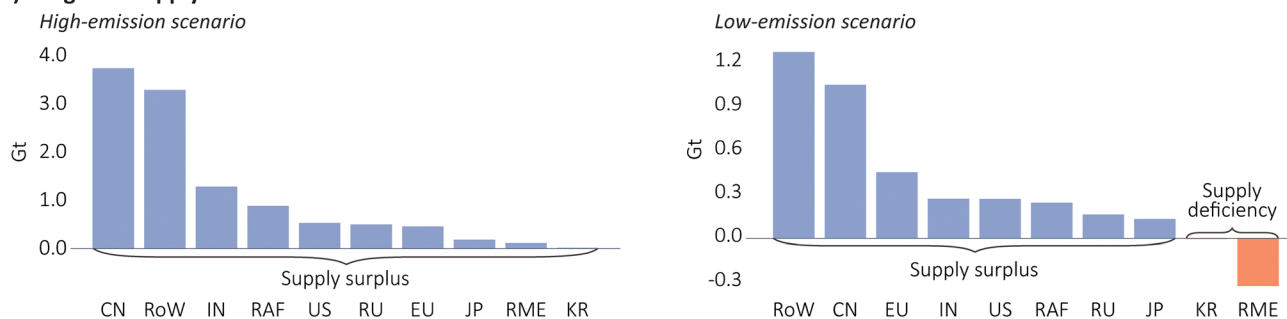
The GHG savings and PM-related health impacts of capturing 1 kg CO<sub>2</sub> depend on the sector from which carbon capture is performed. This is because of the different CO<sub>2</sub> concentrations in the flue gas and the different steam sources and electricity mixes used, as illustrated by the environmental-merit-order (EMO) curves in Fig. 3.

By capturing 1 kg CO<sub>2</sub>, the maximum GHG saving would be 1 kg CO<sub>2</sub>-eq., assuming no additional energy input were required for carbon capture. Considering GHG emissions from the additional energy inputs, the actual GHG savings due to carbon capture from the different sectors would be between 0.6 and 0.9 kg CO<sub>2</sub>-eq per kg CO<sub>2</sub> captured on a global average. As a trade-off, between 1 and  $5 \times 10^{-8}$  disability adjusted life years (DALY) per kg CO<sub>2</sub> captured PM-related health impacts would be attributed to carbon capture. If CO<sub>2</sub> emissions in 2050 were captured to the full capacity, 12 000–33 000 DALYs would be lost every year because of PM-related health impacts, which corresponds 0.06–0.17% of the global total PM-related health impacts in 2019.<sup>57</sup>



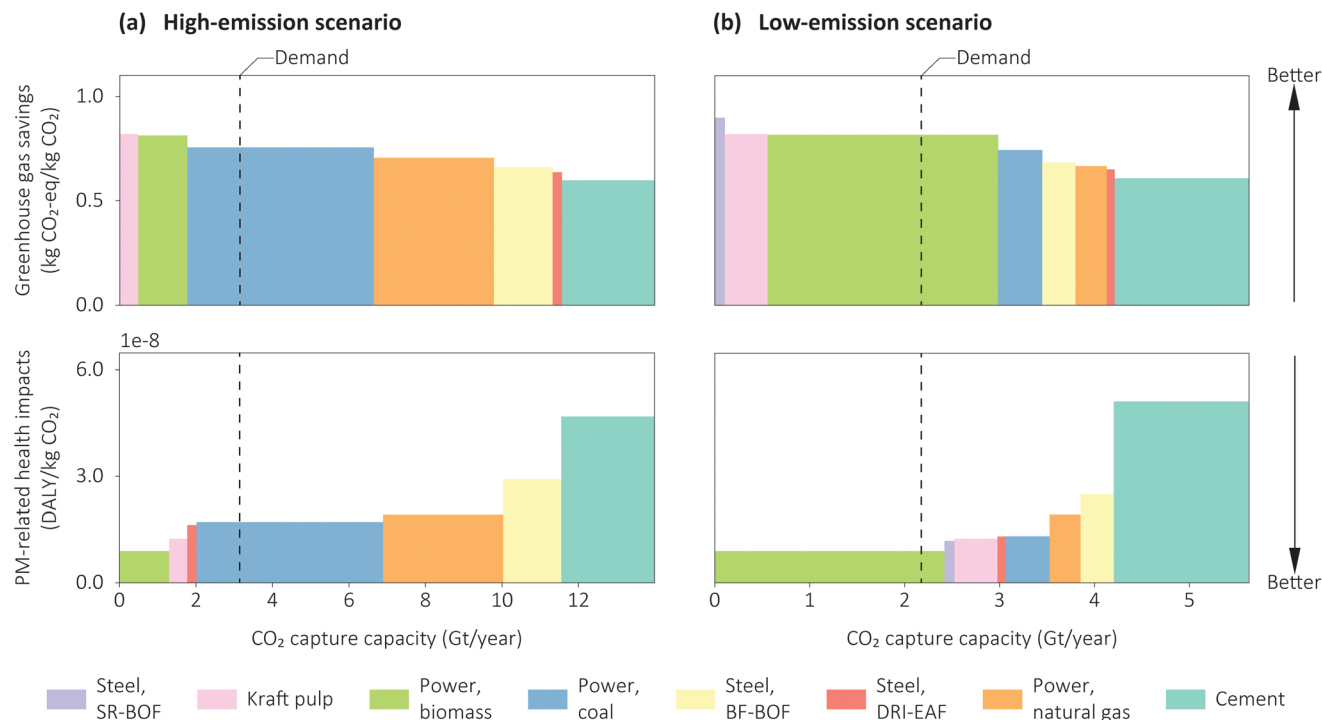
(a) CO<sub>2</sub> Mass flow (unit: Gigatonne)

## (b) Regional supply-demand balance



**Fig. 2** (a) Estimated global CO<sub>2</sub> mass flow under the high- and low-emission scenarios (note the mass flows are differently scaled under the two scenarios). (b) Regional CO<sub>2</sub> supply-demand balance under the high- and low-emission scenarios. Abbreviations: CN, China; EU, the European Union; IN, India; JP, Japan; KR, the Republic of Korea; RAF, Region Africa; RME, Region Middle East; RU, Russian Federation; US: the United States of America; RoW: Rest of the World; BF-BOF, blast furnace-basic oxygen furnace; DRI-EAF, direct reduced iron-electric arc furnace; SR-BOF, smelting reduction-basic oxygen furnace.





**Fig. 3** Greenhouse gas savings (top) and PM-related health impacts (bottom) of 1 kg CO<sub>2</sub> captured from different industries, calculated with global average impact factors, plotted against the maximum global sectoral CO<sub>2</sub> supply capacity (the dashed line indicates the maximum CO<sub>2</sub> demand from the chemical industry) under (a) high-emission scenario and (b) low-emission scenario. Abbreviations: BF-BOF, blast furnace-basic oxygen furnace; DRI-EAF, direct reduced iron-electric arc furnace; SR-BOF, smelting reduction-basic oxygen furnace.

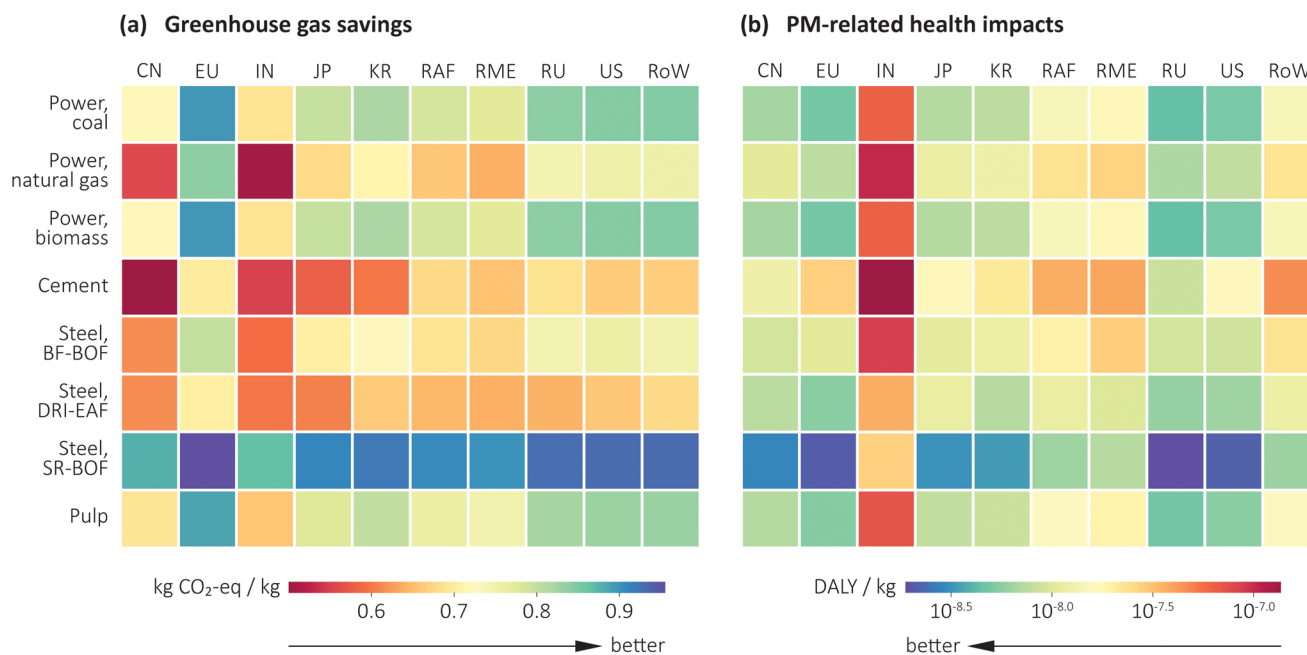
The GHG savings and PM-related health impacts of carbon capture are dominated by the amount and type of energy that needs to be additionally fed into the system. Generally speaking, higher CO<sub>2</sub> concentration in the flue gas would lead to a lower energy requirement for carbon capture. An extreme example is SR-BOF mills, where CO<sub>2</sub> concentration in the flue gas is close to 100%. In this case, only 0.15 kW h electricity per kg CO<sub>2</sub> captured is required for the compression.<sup>33</sup> As a result, with 0.90 kg CO<sub>2</sub>-eq. GHG savings and  $1.19 \times 10^{-8}$  DALY PM-related health impacts per kg of CO<sub>2</sub> captured, SR-BOF steel mills are one of the most preferred CO<sub>2</sub> source under the low-emission scenario. However, SR-BOF steel mills are only assumed to be in place under the low-emission scenario due to its low TRL today, and their maximum CO<sub>2</sub> supply capacity remains low.

Other preferred CO<sub>2</sub> suppliers with low carbon capture-related environmental and health impacts and large supply potential include biomass-fired power plants. This is because we assume that for power plants, the environmental and health impacts of carbon capture come from the regional electricity grid mix to compensate for the power loss due to carbon capture (see section 2.2). Biomass-fired power plants have higher CO<sub>2</sub> concentrations in the flue gas than natural gas-fired power plants, leading to less power loss. In addition, biomass-fired power plants have a large share in the EU, where the electricity grid mix has one of the lowest impact factors, further reducing the impacts of carbon capture from them.

Fig. 4 shows that the impacts of carbon capture also have a strong regional pattern. This is mainly due to the different impact factors of the regional energy mix (Tables S45 and S46 in ESI†). Carbon capture in the EU can yield the most GHG savings with the lowest PM-related health impacts in most cases, thanks to its relatively clean electricity and fuel mix. Least savings in GHG emissions would be achieved by carbon capture in China and India as the result of their high dependency on coal in the fuel mix. Due to major advances in PM-emission control in the Chinese power plants and the overall high PM emissions from a broad range of other sources in the region,<sup>37</sup> the carbon capture-induced relative PM-related health impacts in China are estimated to be comparable to other regions with lower pollution levels such as the EU. In contrast, in India, strict emission control of sulfur dioxide and nitrogen oxides in the industry<sup>37</sup> is lacking, causing carbon capture also having the highest PM-related health impacts among the nine countries/regions investigated. These tendencies depend strongly on the regional background pollution and the emission regulations in 2050, and are thus subject to major uncertainties.

**3.2.1 Sensitivity analysis: electricity and steam sources.** Since the environmental and health impacts of carbon capture comes mainly from the associated energy consumption, the EMO curves vary when using different energy mixes (Fig. S2–S5 in ESI†). For electricity, besides the regional grid mix in 2019 as in the base case (Fig. 3 and 4), we also examined scen-





**Fig. 4** Heat map of (a) greenhouse gas savings and (b) PM-related health impacts of capturing 1 kg CO<sub>2</sub>, by supply sector and region. Abbreviations: CN, China; EU, the European Union; IN, India; JP, Japan; KR, the Republic of Korea; RAF, Region Africa; RME, Region Middle East; RU, Russian Federation; US: the United States of America; RoW: Rest of the World; BF-BOF, blast furnace-basic oxygen furnace; DRI-EAF, direct reduced iron-electric arc furnace; SR-BOF, smelting reduction-basic oxygen furnace.

arios with the projected regional grid mix in 2050 with and without full CCUS deployment. The impacts associated with carbon capture are lower when using the projected electricity grid mix in 2050, both with and without CCUS. The sectoral rankings in the EMO curves are not significantly affected, with the exceptions noted for the electricity grid mix with full CCUS development under the low-emission scenario. In this case, thanks to the carbon capture at biomass-fired power plants, higher electricity demand would lead to higher savings in GHG emissions, which is counter-intuitive. However, net-negative biomass electricity may not be an unlimited good due to the availability of suitable biomass, associated costs and other impacts of biomass-fired power plants, and all these factors should be assessed in future studies.

Besides using mixed-fuel boilers, the steam for MEA regeneration in cement kilns and steel mills can also be produced with natural gas boilers or electrode vessels. When natural gas is used as the fuel for steam generation, the ranking of cement kilns in EMO curves would be improved, especially when combined with the electricity grid mix in 2019. Scenarios of using electrode vessels to produce stream would have the lowest carbon footprint of all MEA regeneration options when the electricity grid mix is decarbonized.

### 3.3 Bottom-up case studies: optimizing the CO<sub>2</sub> supply to chemical manufacturing sites in China and the Middle East

**China:** The priority rankings of the four types of CO<sub>2</sub> sources in the EMO curve for China are the same, in terms of both GHG savings and PM-related health impacts: coal-fired power

plants are the most preferred suppliers, followed by BF-BOF steel mills, natural gas-fired power plants, and cement kilns (Fig. 5a and b).

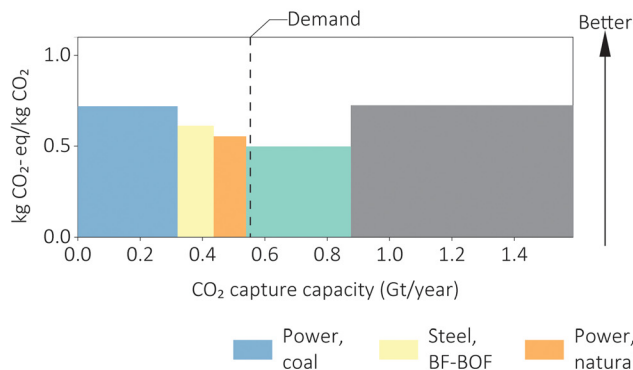
However, in the supply-chain optimization where the impacts of truck transportation of CO<sub>2</sub> are additionally considered, the results by minimizing the total GHG emissions (Fig. 5c) and by minimizing the total regional PM-related health impacts (Fig. 5d) are different. As a general pattern, the transportation distance is longer when minimizing the total regional climate change impacts (average transportation distance being 224 km) than when minimizing the total regional PM-related health impacts (average transportation distance being 182 km). For example, when minimizing the total regional PM-related health impacts, a local cement kiln would be chosen as the CO<sub>2</sub> supplier instead of a coal power plant if located more than 228 km away (break-even distance). When minimizing the total regional climate change impacts, this break-even distance becomes 1282 km. Overall, truck transportation accounts for 7–9% of the total climate change impacts and 32–38% of the total PM-related health impacts in the value chain of carbon capture and transportation (Table S53 in ESI†).

**3.3.1 Sensitivity analysis 1: CO<sub>2</sub> transportation using pipelines.** When pipelines were used for CO<sub>2</sub> transportation in China, the transportation distance would be longer in general (average distances being 227–233 km) because of the relative smaller impacts from pipeline transportation in comparison to truck transportation (Fig. S6 and Table S54 in ESI†). The coal power plants would still be more preferred than the cement kilns in terms of savings on climate change impacts

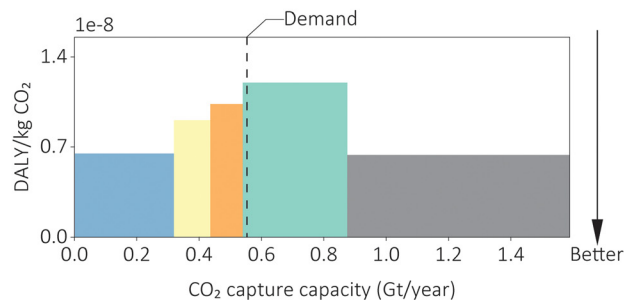


## Environmental-merit-order curves of carbon capture

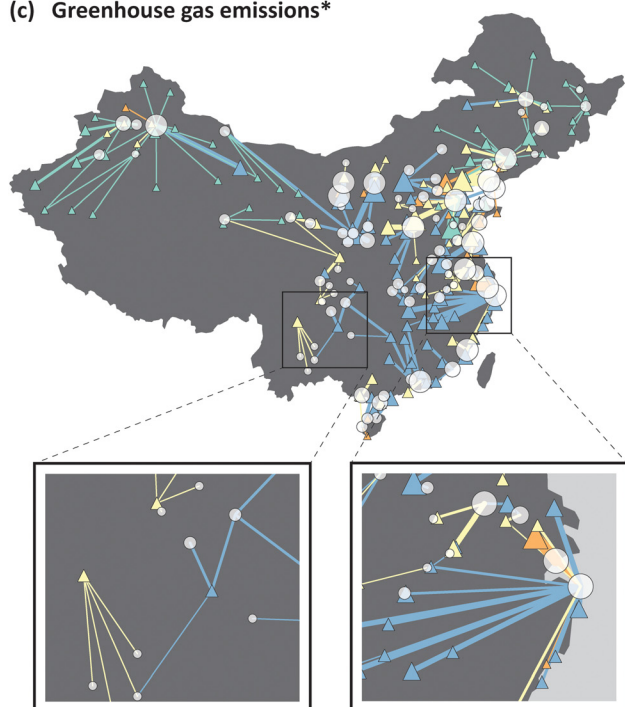
## (a) Greenhouse gas savings\*



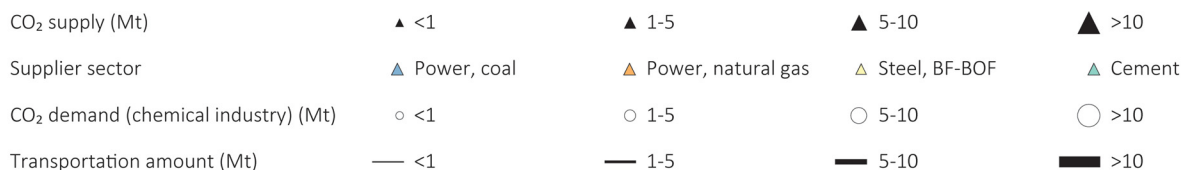
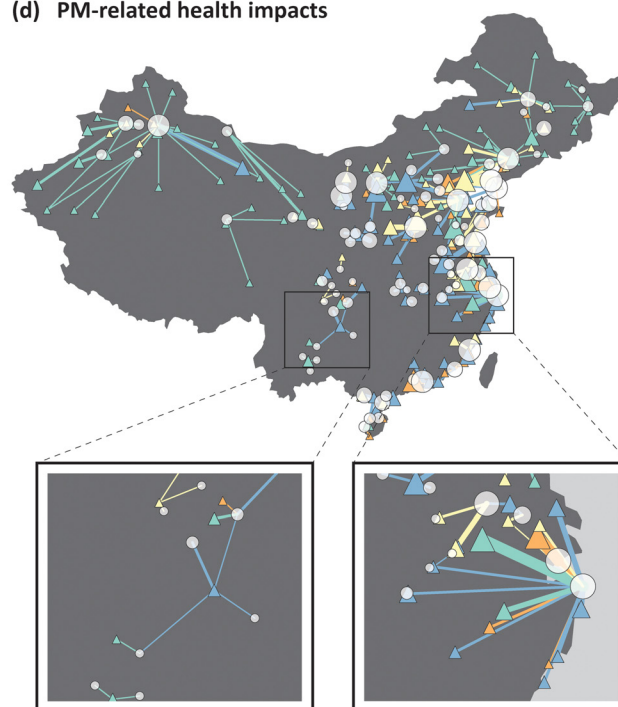
## (b) PM-related health impacts

CO<sub>2</sub> supply chain optimization by minimizing

## (c) Greenhouse gas emissions\*



## (d) PM-related health impacts



**Fig. 5** (a) and (b): GHG savings and PM-related health impacts of carbon capture from different sectors in China. (c) and (d): CO<sub>2</sub> supply chain optimization in China under the low-emission scenario in 2050 by minimizing the total regional climate change impacts and the total regional PM-related health impacts. Zoomed-in areas represent examples of major differences between the two strategies. Abbreviations: BF-BOF, blast furnace-basic oxygen furnace.\* GHG emissions of carbon capture = captured CO<sub>2</sub> amount – GHG savings.

even if they were located 3102 km farther than the cement kiln. This break-even distance would become 4802 km when considering the PM-related health impacts. As a result, total climate change impacts and total PM-related health impacts due to carbon capture and transportation in China would be

reduced by 6–9% and 34–36%, respectively, when pipelines were used for CO<sub>2</sub> transportation in comparison to the basic scenario to fulfill the demand from the chemical industry.

**3.3.2 Sensitivity analysis 2: biomass-fired power plants as additional CO<sub>2</sub> suppliers.** Biomass-fired power plants are



among the most preferred CO<sub>2</sub> suppliers in China, with its low carbon capture-related impacts and large potential capture capacity under the low-emission scenario. Assuming truck transportation, when minimizing the total climate change impacts, all of the CO<sub>2</sub> demand from the chemical industry would be supplied by nearby solid biomass- or coal-fired power plants, with an average transportation distance of 170 km (Fig. S7 and Table S55 in ESI†). When minimizing the total PM-related health impacts, more local suppliers of other types would be used and the average transportation distance would become 131 km. Still, solid biomass- and coal-fired power plants would account for 86% of the CO<sub>2</sub> supply to the chemical industry. Overall, when biomass-fired power plants were considered as additional CO<sub>2</sub> suppliers to the chemical industry in China, total climate change impacts and total PM-related health impacts due to carbon capture and transportation would be reduced by 18% and 24–28%, respectively.

**The Middle East** represents a region with insufficient CO<sub>2</sub> supply under the low-emission scenario in 2050. Only 27% of the demand from the chemical industry could be fulfilled by carbon capture (Fig. 6a), even if it were deployed at the maximum capacity at all the natural gas-fired power plants, DRI-EAF steel mills, and cement kilns. Since all supply sources are utilized to the full capacity, the linear optimization model can only minimize the total transportation distance. As a result, the optimization results by minimizing the total GHG emissions and total PM-related health impacts are the same (Fig. 6b).

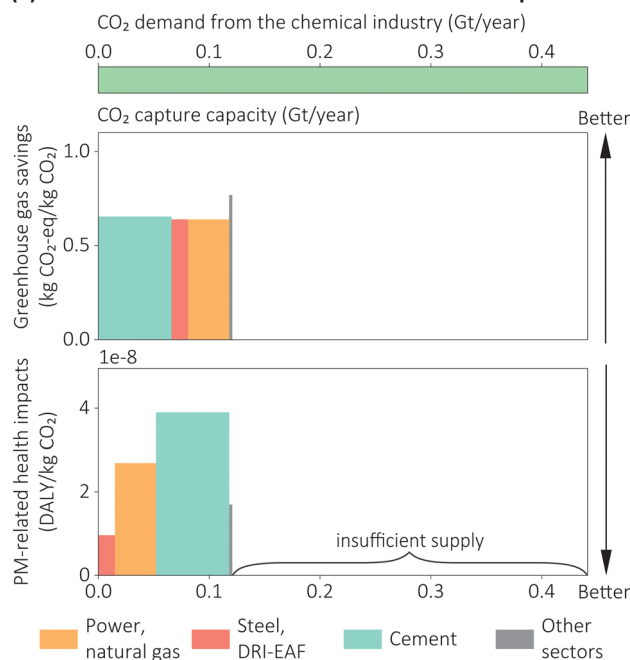
Biogenic electricity production is expected to be deployed in the Middle East in 2050, up to 59 terawatt-hour (TW h) under the low-emission scenario (see Table S15 in ESI†). Since there are only biogas-fired power plants but no solid biomass-fired power plants in the region in 2019,<sup>4</sup> we assumed the biogenic electricity in 2050 would also primarily come from biogas, which was excluded from the scope of carbon capture in this study due to the small average capacity of biogas-fired power plants (described in section S1.1.1 in ESI†). Even if we assume all 59 TW h biogenic electricity would come from solid biomass with another 50 Mt of CO<sub>2</sub> supply (as calculated with global average fuel efficiency under the low-emission scenario in 2050), only 40% of the feedstock demand from the chemical industry could be covered with local CO<sub>2</sub> supply.

## 4. Discussion

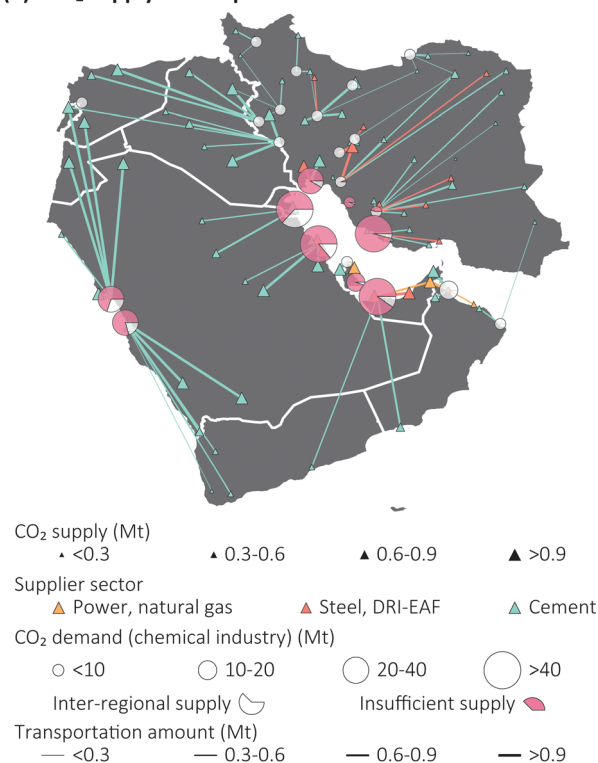
### 4.1 Feasibility of a CO<sub>2</sub>-based chemical industry

The two scenarios explored in this study provide insights into the potential maximum and minimum range of CO<sub>2</sub> emissions in 2050. We estimate the global maximum CO<sub>2</sub> capture capacity from power plants, cement kilns, steel mills, and kraft pulp mills in 2050 to be between 5.6 and 14.0 Gt. Our lower limit (from the low-emission scenario) is slightly lower than IEA's estimation in its net zero emissions scenario (7.6 Gt annual CO<sub>2</sub> capture by 2050, including 1.0 Gt from direct air capture).<sup>58</sup> The main reason for the difference is that we do

### (a) Environmental merit order curves of carbon capture



### (b) CO<sub>2</sub> supply chain optimization



**Fig. 6** (a) GHG savings and PM-related health impacts of carbon capture from different sectors in the Middle East. (b): CO<sub>2</sub> supply chain optimization in the Middle East under the low-emission scenario in 2050. Abbreviations: DRI-EAF, direct reduced iron-electric arc furnace.\* GHG emissions of carbon capture = captured CO<sub>2</sub> amount – GHG savings.



not consider the chemical and refinery industries as potential CO<sub>2</sub> suppliers in this study, as our base assumption is net-zero emissions from the chemical industry.

We further investigate the CO<sub>2</sub>-based production routes of the seven key chemicals that have either been commercialized or are with relatively high TRL as the key pathway to achieve net-zero GHG emissions of the chemical industry. As such, the maximum CO<sub>2</sub> demand from the chemical industry in 2050 are estimated to be between 2.2 and 3.1 Gt. Our result is slightly lower than the estimated 2.8–3.7 Gt global CO<sub>2</sub> demand from a CO<sub>2</sub>-based chemical industry in 2030 by an early study,<sup>49</sup> mainly because they assumed ammonia being also produced *via* a CO<sub>2</sub>-based route.

Globally, our estimates suggest that the feedstock demand from the chemical industry can be well covered by the maximum CO<sub>2</sub> capture capacity. Hence, feedstock availability is not a constraint factor for the transition towards a fully CO<sub>2</sub>-based chemical industry on the global basis. Despite the global abundance of CO<sub>2</sub> supply, certain countries/regions such as the Republic of Korea and the Middle East might still face in-region supply shortage in 2050. A fully-CO<sub>2</sub> based chemical industry in those regions would require more costly options with higher environmental impacts, such as feedstock import from other regions and additional implementation of direct-air-capture facilities.<sup>34</sup>

Furthermore, it is noted that the cost and stable availability of feedstocks usually play an important role in planning the locations of manufacturing sites for bulk chemicals. For example, the traditional petrochemical industry in the Middle East underwent rapid development in the past decades, due to the abundance of the low-cost feedstocks of oil and gas. However, with the intended transition of the chemical industry, the current feedstock advantage in the Middle East would diminish in the future. This indicates the CO<sub>2</sub>-based chemical manufacturing sites might need to be re-positioned based on the regional feedstock supply-demand balance (see section 4.3 below).

#### 4.2 Upscaling carbon-capture projects

While the maximum CO<sub>2</sub> capture capacity is not a constraint for the CO<sub>2</sub>-based chemical industry on the global scale, the speed of actual deployment of carbon-capture projects can limit the large-scale CO<sub>2</sub> utilization. As of 2021, the global operational capacity of carbon capture is 0.04 Gt CO<sub>2</sub> per year.<sup>18</sup> In order to satisfy the need from the chemical industry, the global capacity needs to increase by 55–78 times within the upcoming 30 years. The current main obstacles that limit large-scale deployment of carbon-capture projects in the short to medium term include the technical barrier to lower the energy penalty of carbon capture and the high financial cost. However, a previous study found that CCUS is more cost-effective than other carbon mitigation pathways in the long run,<sup>59</sup> indicating the need for enabling policy to upscale carbon-capture projects.

Our study further demonstrates that EMO curves (Fig. 3) and impact heat maps (Fig. 4) are useful tools to decide which sectors and regions are to be prioritized for carbon-capture

projects. Our priority rankings in terms of GHG emission savings are comparable to the findings by Müller *et al.* for the EU,<sup>35</sup> although the carbon-capture method was not specified in their study. Carbon capture from solid biomass-fired power plants and kraft pulp mills in the EU would bring the highest savings on climate change impacts and incur the least PM-related health impacts. Thus, future carbon-capture projects may first prioritize them by retrofitting these CO<sub>2</sub> point sources. Note that biomass-fired power plants and kraft pulp mills are usually not a major concern as GHG emitters, as they emit mainly biogenic CO<sub>2</sub>. However, as they are identified as the most preferred CO<sub>2</sub> supplier in this study, we highlight that these sectors should target negative CO<sub>2</sub> emissions by capturing biogenic CO<sub>2</sub> to minimize the carbon capture-related impacts of the entire society. In the regions with their electricity grid mixes that have relatively high carbon footprint today, such as India and China, the benefits of GHG savings from carbon capture would be limited. This indicates the need for an energy transition as a prerequisite for making carbon capture more sustainable there.

Chemical absorption with MEA is included in this study as the main carbon-capture method due to its high TRL. It serves as a benchmark in terms of energy penalty and impacts for other capturing methods. Meanwhile, more advanced carbon-capture methods are being developed. For example, the new generation of alkanolamine solvents developed for chemical absorption of CO<sub>2</sub> are able to reduce the steam demand to 2.3 MJ kg<sup>-1</sup> CO<sub>2</sub> captured.<sup>60</sup> Also, membrane-based CO<sub>2</sub> separation is being more widely studied due to its lower energy consumption than conventional carbon-capture methods.<sup>61</sup> With the development of these new technologies, the GHG savings from carbon capture are expected to be higher than estimated in this study.

#### 4.3 Towards net-zero emissions of the chemical industry

In addition to carbon capture, several other factors need to be considered in order to achieve a sustainable CO<sub>2</sub>-based chemical industry. For example, CO<sub>2</sub> transportation between various suppliers and chemical manufacturing sites needs to be carefully planned. Previous studies pointed out that pipeline transportation would be the most economically feasible regional transportation method when CCUS projects are up-scaled.<sup>62</sup> At the moment, the total length of CO<sub>2</sub> pipelines in operation worldwide is only around 8000 km, predominately in the United States for enhanced oil recovery.<sup>63</sup> However, in the China case study, we find that around 70 000 km (linear distance) pipeline network would need to be in place in order to achieve that all existing Chinese chemical manufacturing clusters receive their CO<sub>2</sub> supply *via* pipelines according to the optimization results (Fig. S6 in ESI†). The up-scaling of CO<sub>2</sub> pipeline requires cross-sectoral collaboration, especially regarding early-stage planning of point-to-point match of CO<sub>2</sub> suppliers and consumers.

In this study, we focus on the environmental and health impacts of carbon capture, without considering the impacts of converting CO<sub>2</sub> into chemicals. However, the latter is a necessary step to understand the overall environmental benefits and



trade-offs of a CO<sub>2</sub>-based chemical industry in comparison to the current petrochemical industry. For example, besides CO<sub>2</sub>, hydrogen is also an important feedstock needed for a CO<sub>2</sub>-based chemical industry. Based on the specific hydrogen demand in the individual synthesis routes considered (S1.2 in ESI†), the global hydrogen demand by a CO<sub>2</sub>-based chemical industry in 2050 is estimated to be 344–501 Mt. This translates into 11–17 petawatt-hour (PW h) of electricity demand, taking into account recent research progress that has drastically decreased the electricity consumption of hydrogen production from >50 to 33 kW h kg<sup>-1</sup> H<sub>2</sub>.<sup>64</sup> This electricity demand for hydrogen production corresponds to 50–72% of the world electricity final consumption in 2019.<sup>65</sup> Recent LCA studies have demonstrated that CO<sub>2</sub>-based chemicals such as methanol and ethylene would have lower carbon footprint than their conventional counterparts only when using low-carbon hydrogen, such as green hydrogen from water electrolysis powered with zero- to low-carbon electricity.<sup>66–69</sup> Therefore, speedy upscaling of the capacity of zero- to low-carbon electricity is another pre-requisite for the transition to a fully CO<sub>2</sub>-based chemical industry.

In addition, development of low energy-consuming CO<sub>2</sub>-based chemical production routes is essential. Lowering energy consumption can be achieved through advancements in catalyst development. For example, with mesoporous silver-catalyst, CO<sub>2</sub> fixation of amines can be achieved under room temperature, significantly reducing the energy requirement for the synthesis of *N*-formylated amines.<sup>14</sup> In addition, research is ongoing to directly hydrogenate CO<sub>2</sub> with hydrogen into ethylene, propylene, or BTX aromatics by using selective catalysts.<sup>70,71</sup> If such routes were commercialized and utilized instead of the conventional high-TRL manufacturing routes considered in this study, the total hydrogen demand from a global fully CO<sub>2</sub>-based chemical industry could be reduced by 35%.<sup>49</sup>

In this study, we mainly consider the CO<sub>2</sub>-based production routes for base chemicals, and assume the production of other chemicals would remain unchanged. However, we do acknowledge the rapidly evolving research of CO<sub>2</sub>-based production routes for other chemicals. For example, with metal nanoparticle catalysts or electrocatalysis, carbamate (a specialty chemical of high relevance in pharmaceutical and agrochemical industries) can be synthesized through direct incorporation of CO<sub>2</sub> at mild conditions.<sup>6,72</sup> In addition to the benefits of lowering energy consumption, this novel synthesis route can avoid the use of hazardous reagents as in the traditional production routes, fulfilling the green-chemistry concept.

In addition, in regions with potential supply constraints of CO<sub>2</sub>-feedstock or renewable electricity, CO<sub>2</sub>-based chemical production should be first considered for chemicals with the largest savings on climate change impacts when comparing with the corresponding petrochemicals. A full cradle-to-gate comparative LCA would be necessary as the next step to understand which types of reactions should be prioritized for CO<sub>2</sub> utilization as feedstock.

We acknowledge that many other strategies are being investigated by the chemical industry for its transition to net zero

emissions, including carbon capture at existing chemical manufacturing sites for storage (the CCS pathway), a circular economy with enhanced plastics recycling (the CE pathway), and utilizing biomass as feedstock (the biomass pathway). With the CCS pathway, existing chemical manufacturing sites would be able to continue using their current technology and infrastructure, avoiding the costly stranding of their existing assets.<sup>11</sup> However, net-zero emissions can be hardly achieved with CCS alone because the multiple CO<sub>2</sub> emission points on a chemical manufacturing complex with varied flow rates and CO<sub>2</sub> concentrations make it difficult to capture all emissions from every single stack. In addition, the chemical industry will still be highly dependent on fossil fuels with the CCS pathway.

The CE pathway provides synergies to deal with plastic waste and reduce the virgin feedstock demand for plastic production. However, the benefits of plastics recycling might be curtailed by the low collection rates,<sup>73</sup> limited utilization options for secondary plastics,<sup>74</sup> and hazardous additives used in the plastic production.<sup>75</sup> The theoretical maximum material recycling rate (combined for mechanical and chemical recycling) was assessed to be 70% across all plastic types,<sup>76</sup> yet the best rate of plastic recycling for material use achieved so far is only 24% in Germany in 2019.<sup>77</sup> In addition, the material recycling of other chemical products such as thermosets is even more difficult. Therefore, the role of a circular economy in reducing demand of virgin feedstocks in the chemical industry is projected to remain limited in the foreseeable future.

With the biomass pathway, the electricity demand from plastic production can be reduced by more than 90% in comparison to utilizing CO<sub>2</sub> as the feedstock, but at the expense of more than 40 EJ biomass demand.<sup>76</sup> The availability of future biomass supply from energy crops, wastes and residues, and forestry for material and energy use is highly uncertain with estimations between 107 and 1723 EJ, particularly due to different critical assumptions in crop yield, future population and diet shift.<sup>78</sup> Depending on the type of biomass utilized, various environmental impacts might be incurred as a consequence, such as biodiversity loss, ocean acidification, or eutrophication.<sup>11,79</sup> Therefore, a thorough analysis of using different biomass types as chemical feedstocks is required, taking into account the future biomass availability, TRL of biomass conversion technologies, and environmental impacts from feedstock acquisition and conversion.

Taking into account the pros and cons, previous and our studies suggest that a combination of CCUS and the aforementioned strategies would be needed for transitioning the chemical industry towards net-zero emissions.<sup>76</sup> More in-depth analysis of the three different pathways above and possible combinations, together with CCUS, are warranted to develop the best global and regional net-zero-emission strategies for the chemical industry.

#### 4.4 Towards net-zero emissions of the whole society

This study helps to set priorities regarding where to start capturing CO<sub>2</sub>. To keep the temperature increase within 1.5 °C, it



is imperative to capture CO<sub>2</sub> emissions in almost all sectors and regions in 2050, provided the additional environmental and health impacts associated with carbon capture being not prohibitive.<sup>58</sup> Once reaching such full carbon capture, from the perspective of the whole society, new chemical manufacturing sites can be planned at locations with easy access to CO<sub>2</sub>-feedstock and renewable electricity, regardless of the CO<sub>2</sub> supplying sectors.

Besides the chemical industry, other sectors also rely on CO<sub>2</sub> utilization as a potential low-carbon pathway. For instance, a recent study estimated the potential demand of CO<sub>2</sub> from the fuel sector to be between 0.9 and 3.1 Gt per year in 2050.<sup>80</sup> However, when used as fuel for transportation, CO<sub>2</sub> is released immediately upon combustion. As such, CO<sub>2</sub> emissions are only delayed by days or months, and it is difficult to capture the emitted CO<sub>2</sub> again. Future studies on global and regional CO<sub>2</sub> supply-demand balance need to take its potential utilization in other sectors into consideration as well. Temporally dynamic cradle-to-grave LCAs need to be conducted to compare different potential CO<sub>2</sub> utilization pathways to decide which pathway should be implemented and prioritized to maximize the environmental benefits of carbon capture and utilization.

A successful CCU value chain would need early-stage planning that involves the collaboration across sectors to solve potential conflicts of interest of different stakeholders. One open debate is regarding how to allocate the credits (*e.g.*, GHG savings from carbon capture) and burdens (*e.g.*, PM-related health impacts) related to carbon capture between the CO<sub>2</sub> emitter (*e.g.*, electricity) and the CO<sub>2</sub> consumer (*e.g.*, CO<sub>2</sub>-based chemicals).<sup>35,81,82</sup> In this study, we quantify the total GHG savings and PM-related health impacts from carbon capture from the point view of the society as a whole, and hence, do not need to perform allocation between the CO<sub>2</sub> emitters and consumers.

For future LCA of CO<sub>2</sub>-based chemical products, we propose to continue considering CO<sub>2</sub> as a waste because the main product system (*e.g.*, power plants) would pay for carbon capture as an emission abatement method. In this case, the main product system should get all the credits and burdens related to carbon capture, and the chemical industry gets burden-free CO<sub>2</sub> supply from the power or industrial sectors. This is a different approach from Müller *et al.*,<sup>35</sup> where they considered CO<sub>2</sub> as a valuable product, and hence, CO<sub>2</sub>-feedstock should be credited for the avoided CO<sub>2</sub> emissions using the substitution approach. Their approach means that the power plants or cement kilns cannot reduce or avoid CO<sub>2</sub> emissions with the CCU (since the credit of the reduction goes to the user of CO<sub>2</sub>). However, we would argue that the CCS approach is a case of waste treatment, and the main product would be credited for CO<sub>2</sub> removal. Similarly, CCUS could be considered to be a waste treatment method so that it will not make a difference for the main product system in terms of environmental and health impacts whether the captured CO<sub>2</sub> is for storage or utilization. In other words, our recommendation is to ensure the methodological consistency of allo-

cation in LCA among different downstream mechanisms of carbon capture. In addition, to reach net-zero emissions of the whole society, more CO<sub>2</sub> needs to be captured than demanded from the chemical industry. In this sense, it should not make a difference for the chemical industry which industrial CO<sub>2</sub> source they utilize.

Furthermore, some researchers argue that a focus on CO<sub>2</sub> utilization instead of storage may cause costly distractions from climate change mitigation to reach net-zero GHG emissions because it does not guarantee the net removal of CO<sub>2</sub>.<sup>83</sup> However, CCU could help reduce the challenge of limited regional CO<sub>2</sub> storage capacity that CCS faces, especially in India and China.<sup>28</sup> Additionally, increased implementation of CCU and circular chemical use can help the chemical industry to move away from the reliance on fossil fuel.

#### 4.5 Uncertainties and sensitivity analysis

The uncertainty of CO<sub>2</sub> supply and demand in 2050 is addressed by using a worst-case high-emission scenario and a best-case low-emission scenario to capture the possible range. Under the both scenarios, we find that the CO<sub>2</sub>-feedstock demand from the chemical industry can be well covered by the CO<sub>2</sub> supply on the global average.

The environmental and health impacts of carbon capture are sensitive to the choice of electricity and fuel mixes. When the electricity grid mix were decarbonized, using steam generated in electrode vessels for MEA regeneration would provide the largest GHG savings. However, with the current electricity grid mix, natural gas boiler would be recommended for steam generation on the global average because of its lower impacts.

Power systems, such as coal-fired power plants, may also choose to keep the power output from the primary unit constant. In that case, the energy for carbon capture would need to be supplied by additional fuel input into the system. The CCS facility at the Petra Nova power plant in the US (currently suspended), for example, built a 75-megawatt auxiliary gas turbine to supply electricity and steam for the capture unit.<sup>84</sup> However, since CO<sub>2</sub> from the gas turbine is not captured, the overall rate of CO<sub>2</sub> emissions with the Petra Nova model was found to be more than twice as high as with the Boundary Dam model that does not rely on additional fuel source for the energy supply to the capture unit.<sup>85</sup>

When planning future point-to-point CO<sub>2</sub> supply chain, many of the potential emission sources in 2050 could still be unknown, especially for solid biomass-fired power plants and SR-BOF steel mills that are currently not widely deployed. In the sensitivity analysis in the China case study, we assume the to-be-eliminated coal power plants are retrofitted into solid biomass-fired power plants. It might also be a sensible decision to build solid biomass-fired power plants and SR-BOF steel mills as CO<sub>2</sub> suppliers adjacent to chemical manufacturing sites to minimize the cost and impacts of CO<sub>2</sub> transportation.



## 5. Implications

Building on the findings, we would like to highlight the following options as future actions to ensure an effective and efficient systemic low-carbon transition of the chemical industry and the entire society.

(1) Feedstock availability should be taken into account when planning future chemical manufacturing sites. Manufacturing sites of bulk chemicals are usually centralized in regions with easy and low-cost access to feedstocks. With the feedstock transition of the chemical industry from oil and gas to CO<sub>2</sub>, the scale of the chemical industry in regions such as the Middle East would be expected to shrink due to insufficient local feedstock supply. This could be less ideal for the region's economic development, and corresponding measures need to be considered to mitigate such negative impacts (e.g., by transitioning from large-scale production of low-price base chemicals to smaller-scale production of high-price chemicals). On the contrary, the development of the chemical industry in China was constrained by the availability of oil and gas in the past. With the highest CO<sub>2</sub> supply potential, the chemical industry there could be further developed. Before such expansion takes place, it is key to ensure the availability low-impact electricity grid mix in China.

(2) Low-impact energy mix is fundamental before the large-scale deployment of CCUS projects. Enormous heat and electricity demand is expected from the CCUS value chain: from CO<sub>2</sub> capture and compression, to transportation, and to produce hydrogen as co-reactants. Therefore, to ensure the largest savings on climate change impacts with the least additional other impacts, it is essential to prioritize low-impact energy mix. This implies that the immediate priority for China and India should be to increase the share of renewable energy in their electricity grid mix to make the CCUS value chain more sustainable.

(3) Strategic cross-sectoral planning is key to minimizing the total environmental impact for the whole society to achieve net-zero GHG emissions. In recent years, all sectors are developing their own net-zero-emission pathways. For example, many coal-fired power plants are considering being retrofitted into solid biomass-fired power plants, as a pathway to reduce their greenhouse gas emissions while avoiding the need of carbon capture.<sup>86</sup> However, our analysis reveals that larger cross-sectoral co-benefits from carbon capture can possibly be achieved and should be strived for. Among others, solid biomass-fired power plants should be prioritized for CCUS projects because of its lower carbon capture-related environmental impacts. We call on policy makers and industrial stakeholders to establish open and transparent dialogues and benefits-sharing mechanisms to foster such cross-sectoral collaborations.

## Author contributions

J. H. conceived the idea, collected and processed data, and wrote the manuscript. Z. W. conceived the idea, assisted with

research, and edited the manuscript. C. O. modelled the regionalized PM-related health impacts, and assisted with data collection and manuscript editing. G. G.-G. assisted with research and manuscript editing. S. H. supervised the project, assisted with research and manuscript writing.

## Conflicts of interest

The authors declare no conflict of interest.

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