# SUPPORTING INFORMATION

# Cost Analysis of Carbon Capture and Sequestration of Process Emissions from the U.S. Industrial Sector

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#### **Carbon Capture Retrofit Opportunities for the Industrial Sector**

Many industrial emitters rely on the grid to meet their electricity needs. In 2018 it was reported that the total energy consumption of the U.S. was 3.95 trillion kilowatt-hours (kWh), with the industrial sector comprising roughly 1.09 trillion kWh (i.e., 27.6%). When these indirect emissions from electricity generation are included, the industrial sector is responsible for roughly 30% of total U.S. carbon emissions.<sup>1</sup> Of this energy, 0.14 trillion kWh were generated by industrial facilities with the remaining 0.95 trillion kWh sourced from the electrical grid indicating that 87.2% of industrial electricity comes from the U.S. electrical grid and only 12.8% is from on-site generation.<sup>2</sup> Since the majority of industrial emissions sources rely on the grid to meet their electricity needs, the indirect emissions associated with each industrial facility under consideration have not been included. Additional emissions from industry are the result of stationary combustion onsite at the industrial emissions source. These emissions are associated with equipment such as boilers, heaters, furnaces and kilns, as well as other equipment that combusts carbon bearing fuels or waste stream materials.<sup>3</sup> These emissions have also been subtracted from the total  $CO_2$  footprint of each individual facility in the industrial sector. Subtracting out the indirect and stationary combustion emissions from the total footprint of a given plant allows for focus solely on the chemical process emissions generated on site at the facility. These are the emissions that the facilities have immediate control over and should be those used in determining the potential opportunity for avoiding  $CO_2$  from the industrial sector, in addition to their subsequent qualification potential of the federal tax credit 45Q.

#### **Emissions Considered from the Industrial Sector**

The Environmental Protection Agency (EPA) reports 1,407 industrial facilities emitting 617  $MtCO_2$ -eq in 2017 in the contiguous U.S. in the following sectors: refineries, chemicals, minerals, metals, and pulp & paper. This paper aims to outline best opportunities for point source carbon capture from industrial exhausts and provide insight on capture potential of difficult-to-avoid emissions. This requires focusing on large process emission exhausts that are not already used for  $CO_2$  supply. For these reasons, facilities supplying  $CO_2$  were excluded from the dataset, as well as stationary combustion emissions from all facilities and emissions from landfills. Ethanol facilities are good opportunities for point source capture as they emit high purity streams of  $CO_2$ . Data were

compiled from the NEO, EIA, EPM, and RFA<sup>4–7</sup> to complete the EPA dataset regarding the CO<sub>2</sub> emissions from the ethanol production process.

Data provided by EPA combined with the bioethanol database total 1,529 facilities emitting roughly 606 MtCO<sub>2</sub>-eq/yr in total when excluding suppliers of CO<sub>2</sub>, and 1,015 facilities emitting roughly 297 MtCO<sub>2</sub>-eq/yr from industrial processes. The industrial processes occurring in these facilities are discussed in greater detail later in this study in order to estimate what share of the emissions may actually be captured and ultimately the facilities that may benefit from the federal tax credit.

#### **Cost Model**

A technology-agnostic cost model is used in the current work for estimating the costs of  $CO_2$ capture for single-stream systems and is based on a previous model that was developed by the authors.<sup>8</sup> In particular, the cost model for carbon capture is not intended for mixed streams of a given facility since the approach of mixing streams to maximize capture potential would inevitably lead to increased capital due to the additional piping and retrofitting required for such an effort. Although not considered in the current work, mixed streams deserve exploration in order to maximize the avoided emissions of a given facility in addition to increasing a facility's ability to qualify for the federal tax credit 45Q. Due to the variability in both CO<sub>2</sub> feed concentrations and the flow rates of given streams, the model does not focus on any single capture technology. It is anticipated that the industrial sector will have the option to employ a range of separation technologies, from chemical solvent and solid sorbents for the more dilute streams, membranes for the intermediate streams, and potentially simple approaches such as cryogenic separation or compression for higher CO<sub>2</sub> concentration streams or simply streams containing mixtures of CO<sub>2</sub> and H<sub>2</sub>. In addition, the small scale of some of the capture opportunities, may provide excellent entry points for newer technologies where demonstration and deployment is on the scale of capturing a few thousand tonnes of  $CO_2$  per year as opposed to the millions of tonnes per year required for a given facility in the power sector.

The cost model applied in this study is built from data collected from the Integrated Environmental Control Module IECM platform. The IECM provides the cost of CO<sub>2</sub> avoided based on the following:<sup>9</sup>

$$Cost of CO_2 Avoided = \frac{(LCOE)_{CCS} - (LCOE)_{REF}}{\frac{tCO_2}{kWh(REF)} - \frac{tCO_2}{kWh(CCS)}}$$
Eq.1

where LCOE is the levelized cost of electricity for the CCS plant and reference (REF) plant, and the denominator takes into account CCS and reference plant emission rates. To examine the sensitivity of the cost of CO<sub>2</sub> avoided to flow rate (e.g., plant size), the plant size can be adjusted in IECM to a desired nameplate capacity ( in the case of coal-fired plants) or by adjusting the number of turbines and/or turbine design in the case of NGCC. Accordingly, the LCOE and plant emission rate will change, and the cost of CO<sub>2</sub> avoided can be inventoried at a spectrum of flow rates designed to mimic the lower range in volume of CO<sub>2</sub> captured in industrial facilities. Likewise, understanding the influence of percent capture can be achieved by manually adjusting the percent capture in the IECM sub-menus. More importantly, and central to the study, is an understanding of the influence of CO<sub>2</sub> purity on the cost of CO<sub>2</sub> avoided. Here, since CO<sub>2</sub> purity is not directly adjustable, costs were inventoried for NGCC capture (approx. 4.2% CO<sub>2</sub> v/v), pulverized coal capture (approx. 12% CO<sub>2</sub> v/v) and integrated gasification combined cycle (approx. 37% CO<sub>2</sub> v/v). Altogether, these results were fit in a multi-regression model to produce the following:

Cost of  $CO_2$  Captured  $(C_{ca}) = 10^{(2.18-0.426*log\alpha-0.391*log\beta-0.028*log\gamma)}$  Eq.2 where  $\alpha$  is the capture rate,  $\beta$  is the CO<sub>2</sub> concentration, and  $\gamma$  is the volumetric flow rate in tonnes/day.

To obtain the total cost of CO<sub>2</sub> avoided, one must add in the cost of compression, transport and injection, and re-levelize the cost to account for any direct, indirect or embodied emissions over the entire lifecycle. Compression is calculated based on the methodology outlined by McCollum and Ogden and others.<sup>10,11</sup> Liquefaction costs are calculated assuming conditions of 1.7 MPa and -30 °C.<sup>10</sup> Compression for pipeline is calculated assuming 10 MPa using 5 stages and inter-stage cooling, compression ratio of 1.76 and isentropic efficiency of 0.75. The approximate energy for compression (including cooling) is 111 and 140 kWh/tCO<sub>2</sub> for trucking and pipeline, respectively. For trucking, additional compression prior to injection results in an additional energy of 41

kWh/tCO<sub>2</sub>. The levelized cost of compression is calculated by adding the levelized amortized capital payment, the purchased cost of electricity per tonne CO<sub>2</sub> compressed, and an:

$$C_{co,i} = \frac{TCC_{comp,i} * (CRF + O\&M)}{nCO_2} + w_{co,i} * C_E$$
Eq.3

where  $TCC_{comp,i}$  is the total capital cost of the compression/pumping system, *CRF* is the capital recovery factor, *O&M* is an operation and maintenance factor applied to the total capital cost of compression (taken as 0.04 in this study),  $nCO_2$  is the total amount of CO<sub>2</sub> compressed in tonnes per year,  $w_{co,i}$  is the total work for compression and cooling,  $C_E$  is the cost of electricity, and the index *i* indicates a specific transport mode.

The trucking transport model is based largely on the work of Berwick and Farooq,<sup>12</sup> using updated fuel emission rates, fuel costs, and labor costs. Source-end use distances were obtained by performing an origin-destination distance matrix over a U.S. street network dataset. This set of distances together with the estimated  $CO_2$  demand for each end use served as model inputs. The levelized cost of transport via trucking is calculated from:

$$C_{t_tr} = c_T + w_T + f_T Eq.4$$

where  $c_T$  is the levelized unit cost of capacity per tCO<sub>2</sub> delivered amortized over the useful equipment lifetime (here 5 years per truck and an annual cap of 100,000 miles),  $w_T$  is the timeaveraged variable operating costs (\$/tCO<sub>2</sub>) including fuel, maintenance, tolls and labor, and  $f_T$  is the time-averaged fixed operating costs (\$/tCO<sub>2</sub>) including permits, licenses, and insurance.

Pipeline costs were calculated using the FE/NETL CO<sub>2</sub> transport cost model<sup>13</sup> and the regression model of McCoy and Rubin.<sup>14</sup> Pipelines were assigned for single source-sink pairings where the geodesic source (NG plant)-sink (CO<sub>2</sub> enhanced oil recovery (EOR) or sequestration) distance and pipeline capacity served as model inputs. The levelized cost of transport for pipeline ( $C_{t_pi}$ ) is taken as the first year breakeven cost as calculated in the FE/NETL CO<sub>2</sub> transport cost model.<sup>13</sup>

The cost of injection ( $C_s$ ) is assumed as \$11/tCO<sub>2</sub> for both dedicated geologic sequestration<sup>15</sup> and EOR<sup>16</sup> based on average literature costs for injection and monitoring applied to geologic sequestration and EOR.

The total cost of CO<sub>2</sub> avoided is calculated as:

Cost of CO<sub>2</sub> Avoided 
$$\left(\frac{\$}{tCO_2}\right) = C_{ca} + \frac{C_{co,i} + C_{t_i} + C_s}{(1-x)} - C_q$$
 Eq.5

where the index *i* represents either transport mode,  $C_q$  is any applicable tax credit, and *x* represents the total lifecycle CO<sub>2</sub> emitted over the entire transport chain (excluding capture where those emissions are embodied in  $C'_{ca}$ ), on a tonne emitted per tonne captured basis.

# **Industrial Processes: Chemical Reactions**

**Table S1**. Chemical Reactions Associated with Industrial Process Emissions that Produce CO<sub>2</sub> as a Byproduct

Process	Chemical Reaction	Carbon Source			
Chemicals					
Ammonia <sup>17</sup> Primary Reforming Secondary Reforming Shift Overall	$\begin{array}{c} {\rm CH}_4 + {\rm H}_2 {\rm O} \rightarrow {\rm CO} + 3{\rm H}_2 \\ {\rm CH}_4 + {\rm O} \rightarrow {\rm CO} + 2{\rm H}_2 \\ {\rm CO} + {\rm H}_2 {\rm O} \rightarrow {\rm CO}_2 + {\rm H}_2 \\ 0.88{\rm CH}_4 + 1.26{\rm air} + 1.24{\rm H}_2 {\rm O} \rightarrow 0.88{\rm CO}_2 + {\rm N}_2 + 3{\rm H}_2 \end{array}$	Methane (Natural Gas)			
Bioethanol 18	$C_6 H_{12} O_6 + yeast \rightarrow 2C_2 H_5 OH + 2CO_2 + Heat$	Sugar			
Hydrogen <sup>19</sup> Steam Reforming Water-Gas Shift	$CH_4 + H_2O \rightarrow CO + 3H_2$ $CO + H_2O \rightarrow CO_2 + H_2$	Methane (Natural Gas)			
Refining Fluid Catalytic Cracking <sup>20</sup>	$\begin{array}{c} \mathrm{CH}_{1.33}\mathrm{O}_{0.43} + 0.26\mathrm{O}_2 \rightarrow 0.65\mathrm{CH}_{1.12} + 0.27\mathrm{H}_2\mathrm{O} + 0.34\mathrm{CO}_2\\ \mathrm{Heavy}\ \mathrm{Cycle}\ \mathrm{Oil} \rightarrow \mathrm{Gasoline}\\ \mathrm{Heavy}\ \mathrm{Cycle}\ \mathrm{Oil} \rightarrow \mathrm{Gas}\\ \mathrm{Heavy}\ \mathrm{Cycle}\ \mathrm{Oil} \rightarrow \mathrm{Coke}\\ \mathrm{Light}\ \mathrm{Cycle}\ \mathrm{Oil} \rightarrow \mathrm{Gas}\\ \mathrm{Light}\ \mathrm{Cycle}\ \mathrm{Oil} \rightarrow \mathrm{Gas}\\ \mathrm{Light}\ \mathrm{Cycle}\ \mathrm{Oil} \rightarrow \mathrm{Gas}\\ \mathrm{Light}\ \mathrm{Cycle}\ \mathrm{Oil} \rightarrow \mathrm{Coke}\end{array}$	Long-chained hydrocarbons			
Metals					
Aluminium Production <sup>21</sup>	$2\text{Al}_2\text{O}_3 + 3\text{C} \rightarrow 4\text{Al} + 3\text{CO}_2$	Coking Coal			
Ferroalloys <sup>22</sup>	$Fe_2O_3 + SiO_2 + 7C \rightarrow 2FeSi + 7CO$ $Fe_2O_3 + 2MnO + 5C \rightarrow 2FeMn + 5CO$ $Fe_2O_3 + 2CrO + 5C \rightarrow 2FeCr + 5CO$	Coking Coal Coking Coal Coking Coal			
Iron & Steel <sup>23</sup> Coke Lime Production	$Fe_{2}O_{3} + 3CO \rightarrow 2Fe + 3CO_{2}$ $Fe_{2}O_{3} + 3C \rightarrow 2Fe + 3CO$ $C + O_{2} \rightarrow CO_{2}$ $CO_{2} + C \rightarrow 2CO$ $CaCO_{3} + Heat \rightarrow CaO + CO_{2}$	Coking Coal Coking Coal Coking Coal Carbonate			
Stag Formation	$\frac{1}{1} \cos(1 - \frac{1}{2}) \cos(1 - \frac{1}{$				
Cement Production <sup>24</sup>	$CaCO_{a} + Heat \rightarrow CaO + CO_{a}$	Carbonate			
Alkaline Oxides (Lime) <sup>25</sup>	$Ca/MgCO_2 + Heat \rightarrow Ca/MgO + CO_2$	Carbonate			
Glass <sup>26</sup>	Various Components + Heat $\rightarrow$ Glass + CO <sub>2</sub>	Carbonate			
Others					
Pulp & Paper <sup>27</sup> <i>Lime Production</i>	Wood Organics $+ O_2 \rightarrow CO$ CaCO <sub>3</sub> $+$ Heat $\rightarrow$ CaO $+$ CO <sub>2</sub>	Carbonate			

#### **Emissions of Industrial Sectors Considered**

The EPA reports 1,407 industrial facilities emitting 617 MtCO<sub>2</sub>-eq in 2017 in the contiguous United States in the following sectors: refineries, chemicals, minerals, metals, and pulp & paper.<sup>28</sup> Of these facilities, 52 are collectively responsible for 71 MtCO<sub>2</sub>-eq and are also suppliers of CO<sub>2</sub>. These CO<sub>2</sub> producers were discarded from the dataset because the present study aims to quantify opportunities for CO<sub>2</sub> capture where these facilities are already capturing their CO<sub>2</sub>. Emissions due to stationary combustion account for 284 MtCO<sub>2</sub>-eq, and these emissions were also discarded in order to focus specifically on process emissions. Finally, emissions from waste management (i.e., 6 MtCO<sub>2</sub>-eq) were also discarded due to the difficulty in capturing CO<sub>2</sub> emitted from landfills and its low share of the CO<sub>2</sub>-eq emissions from the industrial sector.

Process emissions from the refineries, chemicals, minerals, metals, and pulp & paper industrial sectors totaled to 256 MtCO<sub>2</sub>-eq in 2017 at the 841 facilities that do not supply CO<sub>2</sub>. Facilities were discarded, when emissions from the industrial process make up <1wt% of the total U.S. CO<sub>2</sub> emissions and when the emissions were primarily comprised of a greenhouse gas other than CO<sub>2</sub>, as they cannot be captured with the technology we consider (Table S2). Therefore, the cost analysis of this study focuses on 656 facilities emitting 242 MtCO<sub>2</sub> from their process.

The EPA classifies 171 ethanol facilities as "other" and do not report process emissions from ethanol production. The fermentation process produces over 16 billion gallons of ethanol each year, with CO<sub>2</sub> produced as a byproduct at high purity. In addition to the EPA dataset, additional data regarding bioethanol production in the U.S. were gathered from the Nebraska Energy Office (NEO), the U.S. Energy Information Administration (EIA), the Ethanol Producer Magazine (EPM), and the Renewable Fuel Association (RFA).<sup>4–7</sup> The CO<sub>2</sub> emissions from fermentation were calculated following a method used by Sanchez et al.<sup>29</sup> and described in detail by Hornafius & Hornafius,<sup>30</sup> using the stoichiometric equation for glucose fermentation combined with mass-balance calculations. The total process emissions from the 202 U.S. ethanol plants are 47 MtCO<sub>2</sub>/yr, with 27 ethanol facilities reported as suppliers of CO<sub>2</sub> by the EPA, and with 1 ethanol facility in Decatur, Illinois already capturing and sequestering its CO<sub>2</sub> in a deep saline aquifer.<sup>31</sup> For consistency, and to outline carbon capture opportunities, these facilities were discarded from the dataset with the remaining 174 ethanol plants considered with total process emissions of 41 MtCO<sub>2</sub>/yr (Table 1 in the main text).

Name	Percent of Total Process Emissions	Included?	Reason				
Chemicals							
Petroleum Refining	16.6%	Yes					
Bioethanol	14.4%	Yes					
Hydrogen	11.7%	Yes					
Fluorinated Products	3.2%	No	All process emissions are from hydrofluorocarbons.				
Adipic Acid	2.6%	No	Only emissions from N <sub>2</sub> O				
Ammonia	2.5%	Yes					
Ethylene	1.7%	Yes					
Nitric Acid	1.6%	No	Only emissions from N <sub>2</sub> O				
Carbon Black	1.0%	Yes	• –				
Other Petrochemicals	0.6%	No	Low Percentage, wide array of chemicals				
Titanium Dioxide	0.5%	No	Low Percentage				
Phosphoric Acid	0.3%	No	Low Percentage				
Methanol/Methane	0.3%	No	Low Percentage				
	Me	etals					
Iron and Steel	9.6%	Yes					
Aluminum	0.8%	No	Low Percentage				
FerroAlloy	0.6%	No	Low Percentage				
Lead	0.2%	No	Low Percentage				
Zinc	0.2%	No	Low Percentage				
Magnesium	0.2%	No	Low Percentage				
	Minerals						
Cement	22.5%	Yes					
Lime	5.7%	Yes					
Glass	0.7%	No	Low Percentage				
Soda Ash	0.5%	No	Low Percentage				
Others							
Pulp and Paper	1.88%	No	Minimal availability of process data				
Summary							
Total Emissions Neglected	38.5%						
Emissions Accounted for in Table	99.8%						
All Emissions Being Included	61.3%						

**Table S2**. Percent of Process Emissions from Each Industry in the United States and Rationale for

 Analysis

#### **Descriptions of the Industrial Processes**

Industry	Stationary combustion	Process emissions Unit considered for CO <sub>2</sub> capture			Other process emissions
	CO <sub>2</sub> emissions [wt%]*	Name	CO <sub>2</sub> emissions [wt%]*	CO <sub>2</sub> purity [wt%]	CO <sub>2</sub> emissions [wt%]
Refining**	63	FCC HSU	25 6	15 45	6
Bioethanol	32	Fermenter	68	<b>99</b> + <sup>32</sup>	0
Hydrogen	3	HSU	72	45 <sup>33</sup>	25
Ammonia	26	HSU	42	45 <sup>33</sup>	32
Iron & steel	54	Blast furnace	36	20-25 24	10
Cement	4	Exhaust stack	96	14-33 24,34,35	0

**Table S3**. Breakdown of the emissions and details about the unit considered for  $CO_2$  capture for each type of industrial facility.

\* Percentage of the  $CO_2$  emissions over the total  $CO_2$  emissions from the sector, process emissions from the fermenter in the bioethanol sector and from the exhaust stack in the cement sector represent 100% of the process emissions from these sectors.

\*\* Values averaged over all considered facilities of the refining industry, see Figure S4 for details

#### **Cement Manufacturing**

Cement is produced by grinding mined limestone, followed by several heating steps to remove  $CO_2$  from the limestone to ultimately form calcium oxide as shown in Table S1 and also demonstrated in Figure S1.<sup>36</sup> Here, the CO<sub>2</sub> emissions associated with Portland cement production typically emits ~0.9 tCO<sub>2</sub>/tonne of cement produced.<sup>37</sup> The product exiting the rotary kiln is termed clinker, which is composed of the calcium oxides produced at high temperature. Following the kiln, the clinker may be stored before it is mixed with gypsum and processed in the cement mill to produce the final cement product.<sup>24</sup> The CO<sub>2</sub> emissions associated with cement production are emitted almost entirely through kiln heating fired with natural gas (Table S3). The concentration of CO<sub>2</sub> exiting the kiln may be between 14-33% depending on the composition of the carbonate feedstock and exhaust stream generated from natural gas combustion.<sup>24,34,35</sup>



**Figure S1.** Process flow diagram of conventional cement production process showing the primary exhaust stream with  $CO_2$  concentration that may range between 14-33%. Process emissions comprises of the mixed exhaust streams from preheating, pre-calcination, and the kiln.

#### Bioethanol

Most of the ethanol produced in the U.S. is carried out through the fermentation of corn as shown in Figure S2. The corn goes through a pre-treatment process that enables the extraction of glucose.<sup>38</sup> First, the feed is milled to release the starch components. This is followed by the addition of water and enzymes that convert these components into sugars that can be fermented. Following this pre-treatment, fermentation occurs thereby converting the sugars into bioethanol and CO<sub>2</sub>. This is followed by post-production processing of the bioethanol product before storage. As shown in Table S3, roughly 68% of CO<sub>2</sub> is generated at high purity<sup>32</sup> from the fermenter with nearly 32% of the emissions generated from stationary combustion off-site of the ethanol facility. It is important to note that the emissions reported from stationary combustion may be underestimated since the data are sourced from the EPA database, which reports emissions data for only 144 of the 174 plants (83%) considered in this study. In addition, given that high-purity CO<sub>2</sub> is generated as a byproduct of ethanol production via fermentation, many of the facilities are currently suppliers of commercial CO<sub>2</sub>. More specifically 28 of the 202 ethanol facilities in the U.S. are producers of high-purity CO<sub>2</sub> today, and only the remaining (i.e., 174) plants that are not equipped specifically with CO<sub>2</sub> capture are considered in the current analysis.



**Figure S2.** Process flow diagram of bioethanol production from corn via fermentation. The primary stream contains high-purity  $CO_2$  (99+%) existing the fermenter.<sup>32</sup>

#### Refining

Oil refining is very complex and involves many sub processes that are designed to yield highoctane gasoline in addition to other products and chemicals, including olefins and aromatics such as ethylene, polypropylene, benzene, toluene and xylene. These compounds may be converted to polymers and used commercially in plastics, rubbers and synthetic fibers amongst other applications. Refining conventionally begins with desalting the crude oil for sulfur removal in addition to other impurities.<sup>39</sup> After desalting, the crude oil is sent to a distillation column where the crude oil is fractioned off into liquified petroleum gas, light naphtha, heavy naphtha, kerosene, diesel oil, gas oils, and residue. The residue is further sent to a vacuum distillation unit where the feed is again fractioned into light vacuum gas oil, heavy gas oil, and vacuum residue. Each of these fractions have separate treatment processes to further remove impurities and to produce a saleable product or a high-octane gasoline blend.<sup>39</sup> Among these processes there are many sources of process CO<sub>2</sub> emissions, with the largest source being the fluid catalytic cracker (FCC), which breaks down light vacuum gas oil into olefins, naphtha, and gas oils as demonstrated in Figure S3. In some of the refineries,  $H_2$  production is also carried out and, in these cases, this unit tends to be the major source of  $CO_2$  emissions, followed by the FCC unit. In refineries without H<sub>2</sub> production units, the H<sub>2</sub> is imported by the refinery, instead of being produced on site. Details regarding the

emissions and the units producing the  $CO_2$  are given in Figure S4 and Table S3. The production of H<sub>2</sub> will be discussed in greater detail in the following section with respect to the chemical production, and its production for refining purposes. The FCC process consists of a reaction vessel, fractionator, and regenerator. The reaction vessel is where the catalyst and feedstock react to produce a mixture of olefins, naphtha, and gas oils, which is ultimately sent to the fractionator. The spent catalyst is sent to the regenerator where the accumulated coke is combusted, thereby producing a flue gas containing  $CO_2$  as well as many other compounds.<sup>39</sup>



**Figure S3.** Process flow diagram of the fluid catalytic cracker, which comprises the primary stream of CO<sub>2</sub> emissions associated with refining.



**Figure S4.** Emissions from refining facilities with FCC, FCC and  $H_2$  production, only  $H_2$  production, and neither FCC nor  $H_2$  production, as well as the typical distribution of emissions from each type of refinery.

#### Hydrogen Production

Within the U.S., there are 52 chemical plants associated with  $H_2$  production. These plants comprise 20% of the overall CO<sub>2</sub> emissions associated with chemical production nationwide. Additionally, 39 industrial refining facilities are equipped with the capabilities to produce  $H_2$ onsite. Within the refining industry,  $H_2$  production makes up about 15.5% of process emissions. Considering these two applications,  $H_2$  production amounts to 11.7% of total industrial process emissions.



Figure S5. Process flow diagram demonstrating hydrogen production from steam-methane reforming, currently the most common approach to  $H_2$  production.

The primary method of producing  $H_2$  today is through steam-methane reforming, which is responsible for roughly 95%<sup>40</sup> of the hydrogen used in the U.S. Within this process, methane (natural gas) is reacted with steam under high pressure (i.e., 3-25 bar) and temperature (i.e., 700-1000 °C) conditions in a reformer<sup>40</sup> (Figure S5). This reaction is preceded by a pre-reformer which is used to breakdown some of the larger-chained hydrocarbons contained in natural gas.<sup>41</sup> The products in the reformer are hydrogen and carbon monoxide, which may be further reacted with water via the water-gas shift reaction performed in series in high- and low-temperature shift reactors.<sup>41</sup> Following the shift reactors, the stream undergoes a purification process consisting commonly of a pressure swing adsorption (PSA) system. This system is designed to selectively remove contaminants to produce a high-purity (e.g., 99+%) stream of hydrogen. As a result of the PSA process, the waste stream contains roughly 74% of the process CO<sub>2</sub> emissions emitted from the hydrogen plant facility.<sup>24</sup> The concentration of the CO<sub>2</sub> in the PSA tail gas waste stream following this purification step is 45% with no additional CO<sub>2</sub> purification.<sup>33</sup> However, an additional CO<sub>2</sub> "rinse" step using CO<sub>2</sub>-selective solvents may increase the purity of the CO<sub>2</sub> to 99+%.<sup>33</sup> Additionally, depending on the configuration of the PSA system, CO<sub>2</sub> concentrations between 66% and 94% have also been reported.<sup>42</sup> This being said, a CO<sub>2</sub> concentration of 45% for the hydrogen separation unit (HSU) is assumed in the current analysis.

#### Ammonia Production

Worldwide, ammonia production is estimated to use 1.2% of energy produced and currently comprises 1.2% of global industrial CO<sub>2</sub> emissions.<sup>43,44</sup> Additionally, ammonia production makes up 2.5% of U.S. industrial process emissions. Due to the widespread dependence of ammonia in fertilizers and other applications, it is estimated that over 50% of the nitrogen in the human body is derived from synthetic ammonia, or, namely, the Haber Bosch process.<sup>45</sup>

Industrially ammonia is produced via the Haber process. In this process,  $H_2$  and  $N_2$  are reacted at high temperature (i.e., 400-450 °C) and high pressures (i.e., 200 atm) in the presence of a catalyst.<sup>46</sup> To obtain  $H_2$  for use in this process, most ammonia production facilities have on-site  $H_2$ production that precede the Haber Bosch reaction as shown in Figure S6. Here, methane and steam are fed into the primary reformer. This is followed by a secondary reformer, where air is added to the process. The oxygen in the air is reacts to produce steam, where the nitrogen in air is present in the outlet stream. The stream exiting the secondary reformer is fed into a high temperature shift followed by a low temperature shift to convert the CO to CO<sub>2</sub>. This is followed by a carbon oxide removal step that rids the stream of all CO<sub>2</sub>. The remaining  $H_2$  and  $N_2$  are fed into the ammonia synthesis reactor where it is converted into ammonia. Since the ammonia production itself does not emit CO<sub>2</sub>, the majority of process emissions are sourced from the  $H_2$  production step, that represent 42% of CO<sub>2</sub> emission from ammonia production (Table S3). This  $H_2$  production is consistent with the process outlined in the previous section 'Hydrogen Production'.

As shown in Figure S6, the primary  $CO_2$  emissions source from ammonia production is associated with the H<sub>2</sub> production process, which accounts for roughly 74% of the process emissions associated with ammonia production.<sup>24</sup> Similar to the H<sub>2</sub> production process previously

described, the composition of the produced CO<sub>2</sub> is roughly 45% if a PSA unit is used.<sup>33</sup> However, targeted CO<sub>2</sub> removal via solvents can lead to much higher outlet CO<sub>2</sub> concentrations (99+%). Therefore, facilities that rely on these solvent-based separations will produce CO<sub>2</sub> with higher purity than those using basic PSA units targeting only high purity H<sub>2</sub>. For the purpose of this study, the post-HSU stream is assumed to have a concentration of 45% CO<sub>2</sub> and account for 74% of overall process emissions.<sup>24,33</sup>



**Figure S6.** Process flow diagram for conventional ammonia production, assuming PSA is used in the  $H_2$  production.

#### Iron & Steel Production

The iron and steel production process as illustrated in Figure S7 depicts steel production via the blast furnace (BF) and basic oxygen furnace (BOF). Most of the steel produced in the U.S. is done through a BF-BOF process. In this process, coal undergoes pyrolysis in the coke oven from a coal feedstock, leading to an emissions stream containing  $CO_2$  concentrations from 20%-25%.<sup>24</sup> Some of the coke produced in this process is fed into the sintering unit. Here, iron ore fines, other iron-bearing wastes, and coke dust are fed into a high-temperature reactor. Air is continuously being fed into the reactor and the combustion gases are continuously pulled from the process to a gas cleaning device. This results in a gas stream with concentrations between 5% and 10%  $CO_2$ .<sup>24</sup> The

remaining coke from the coke oven is then combined with sintered ore and limestone in the blast furnace at high temperatures (i.e., >1300°C) to reduce the iron ore, thereby producing pig iron.<sup>23</sup> The molten iron from the BF is then transferred to the BOF along with recycled steel. Here, the feeds react with pure oxygen to remove impurities in the iron to ultimately produce molten steel. This is followed by post-processing of the steel to produce the final product.

In the steelmaking process, the majority of process emissions occur via the blast furnace, which accounts for roughly 78% of the overall process emissions.<sup>24</sup> Additionally, the concentration of  $CO_2$  from the blast furnace ranges between 20-25%,<sup>47</sup> mainly depending on the concentration of limestone and the furnace conditions. Typically, just under 50% of the overall emissions for steelmaking occur from the process, with 36% from the blast furnace itself.



**Figure S7.** Process flow diagram of iron and steel production via the BF-BOF process, with primary  $CO_2$  emissions stream being the blast furnace at 20-25% concentration.



#### Emission reduction potential by industrial sector

**Figure S8.** Emission reduction potential by industrial sector relative to the process emissions and the total emissions considered in the present study.

#### **Enhanced Oil Recovery and Reliable Geologic Sequestration**

The USGS provided shapefiles of the sedimentary basins via the National Assessment of Geologic Carbon Dioxide Storage Resources and the National Oil and Gas Assessments webpages.<sup>48,49</sup> In addition, the USGS has identified 186 storage assessment units (SAU) in 34 basins in the contiguous U.S. A SAU is defined by the USGS as a "mappable volume of rock that consist of a porous reservoir and a bounding regional sealing formation".<sup>50</sup> A method developed by Baik et al.<sup>51</sup> was used to calculate injection rates in sedimentary basins using the radial form of Darcy's law for single-phase flow<sup>52</sup> and the quantitative data assessed by the USGS for 176 SAU in 31 basins.<sup>48</sup> The EOR locations associated with the injection of over 100 ktCO<sub>2</sub>/yr were selected, resulting in 72 injection points out of 101. A previous study carried out by Wilcox et al. describes the EOR and geological sequestration sites in greater detail.<sup>53</sup>



# Carbon hubs in the U.S. and proximity to EOR and geological sequestration

**Figure S9.** Distribution of the industrial facilities identified for  $CO_2$  capture relatively to the sedimentary basins by (a) number of facilities and (b) capture potential.

Location	Distance from sink (miles)	Total number of facilities	Capture opportunities (MtCO <sub>2</sub> /yr)	Number of facilities eligible for 45Q	Facilities eligible for 45Q (MtCO <sub>2</sub> /yr)
Louisiana – Mississippi pipelines	0 - 20	59	24.23	42	23.72
	20 - 50	19	7.45	15	7.31
	50 - 100	12	2.85	7	2.65
Texas-New Mexico pipelines	0 - 20	8	1.97	8	1.97
	20 - 50	13	4.21	11	4.03
	50 - 100	5	0.48	2	0.38
Sedimentary basins	above	276	83.18	176	80.16
	0 - 100	251	77.62	172	74.38
	100 - 200	67	16.98	57	16.50
All contiguous U.S.	-	656	194.93	458	187.74

**Table S4.** Details of the capture opportunities close to the  $CO_2$  pipelines and the sedimentary basins



## Cost breakdown for truck and pipeline delivery

**Figure S10.** Average capture, compression, and delivery costs for (a) trucking transport and (b) pipeline transport of high purity  $CO_2$  from targeted industrial plants to the nearest EOR site (orange bars) or geological sequestration site (blue bars).

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