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Research Article

Mapping Greenhouse Gas Emissions of the U.S. Chemical Manufacturing Industry: The Effect of Feedstock Sourcing and Upstream Emissions Allocation

Qining Chen, Jennifer B. Dunn, and David T. Allen*

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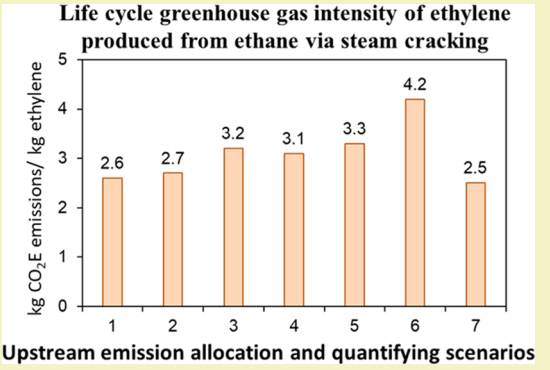
ABSTRACT: Greenhouse gas emissions from 135 commodity chemical manufacturing processes in the United States were estimated based on benchmark process data from U.S. petrochemical manufacturing models. Total greenhouse gas emissions of the 135 processes evaluated are dominated by a small number of process types that have high emission intensities (emissions per mass of product produced) and high production volumes. These processes include facilities for manufacturing ethylene, ammonia, and chlorine. If upstream emissions associated with feedstock sources are included, well-to-gate emission estimates of the chemical manufacturing processes are affected by emission allocation and quantification methods in upstream production, with allocation methods becoming important when the feedstocks are sourced from oil and gas regions that produce multiple products. Well-to-gate emission estimates of ethylene (produced from ethane via steam cracking) and ammonia (produced from natural gas via steam methane reforming) ranged from 2.5 to 4.2 and 1.6−2.9 kg CO_2e/kg production, respectively, depending on how upstream emissions are assigned to natural gas and natural gas liquids feedstocks and how methane emissions are quantified. Accurately characterizing emissions from upstream production of feedstock sources with consistent and transparent metrics is important in identifying potential emission reduction opportunities for chemical manufacturing and for evaluating greenhouse gas benefits arising from recycling of chemical products (e.g., plastics).



KEYWORDS: *Chemical manufacturing, Life cycle assessments, Coproduct allocation, Methane emissions, Oil and gas production, Greenhouse gas emissions*

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INTRODUCTION

The chemical manufacturing industry is one of the most energy intensive manufacturing sectors in the United States, making it a significant source of greenhouse gas emissions. Upstream greenhouse gas emissions and greenhouse gas emissions from chemical manufacturing processes can be assessed in a variety of ways, including analysis of process flowsheets and emission reporting and measurement, such as the reporting done through the Greenhouse Gas Reporting Program (GHGRP).[1] When assessing greenhouse gas emissions and emission reduction potential from the chemical manufacturing industry, most existing studies focus on greenhouse gas emissions from the downstream processes, with less attention paid to upstream feedstock production, in particular, oil and gas production.[2−4]

Oil and gas production, which provides important feedstocks for chemical manufacturing processes, is a major source of methane emissions. Methane is a potent greenhouse gas with a global warming potential (GWP) 84−87 times greater than carbon dioxide over a 20-year period and 28−32 times greater than carbon dioxide over a 100-year period. Global emissions of methane from coal, oil, and natural gas supply chains have been estimated to be approximately 120 Tg/yr.[5] The radiative forcing associated with these methane emissions is approximately 10 000 Tg/yr of carbon dioxide equivalents (CO_2e), assuming a 20-year GWP. This is a warming potential equivalent to the emissions of approximately 2 billion cars, assuming that a typical passenger car emits 4600 kg of carbon dioxide per year.[6]

The magnitude of the methane emissions from coal, oil, and natural gas production and their warming effect have driven a large body of research on the life cycle greenhouse gas emissions of the fuel products of these supply chains, but the impacts of upstream methane emissions on well-to-gate

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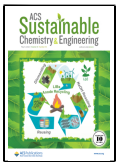

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emissions of chemical products have seen less attention. A challenge in performing these assessments is consistently allocating the emissions of methane among the multiple product streams associated with oil and gas production. Many large oil and gas production regions produce multiple products. For example, in 2019, the Eagle Ford oil and gas production region in the United States had oil production of 1.0 million barrels per day, 0.2 million barrels per day of natural gas liquids (NGLs, primarily ethane, propane, and butane), and 5.8 billion standard cubic feet per day of natural gas.[7] In energy equivalents, this is 6×10^{12} BTU of oil per day, 0.6×10^{12} BTU of natural gas liquids per day, and 6×10^{12} BTU of natural gas per day. The oil, NGLs, and natural gas products are separated in multiple steps at the well head, at gathering sites, and at gas processing plants. Since methane emissions are released at each of these three stages, any life cycle greenhouse gas analysis of the products of oil and gas systems must either explicitly or implicitly assign methane emissions among multiple products.

How emissions are allocated and quantified in upstream oil and gas production can lead to significant differences in emission estimates of upstream oil and gas products. In the Eagle Ford Shale, the differences in emission estimates due to different allocation methods can be as high as 110 CO_2e/MJ of natural gas.[6] Upstream allocation choices can also lead to significant differences in the life cycle emission estimates of downstream chemical production that utilize the oil and gas feedstocks. For example, for hydrogen production from natural gas via steam methane reforming, life cycle emission estimates of hydrogen vary significantly, largely depending on how methane emissions in upstream production are assigned to the natural gas feedstocks.[9,10]

In this work, greenhouse gas emissions from major chemical manufacturing processes in the U.S. are estimated based on process data extracted from the existing U.S. chemical manufacturing models with process utility, stoichiometry and capacity information. Initial estimates were focused on mapping the emissions associated with downstream manufacturing processes and reporting the process-based emission intensities to identify the processes with the highest importance for decarbonization. Two case studies, using ethylene and ammonia production processes from natural gas based feedstocks as examples, were developed to evaluate the impacts of upstream emissions sourcing and allocation choices on the life cycle emission estimates of downstream chemicals. The selected processes have both high emission intensities and high production volumes. Effects of methane emissions vary, depending on the time horizons of the analyses. Methane emissions are more important in near-term horizons, and these effects are also examined in case studies.

MATERIALS AND METHODS

Chemical Manufacturing Processes. The estimates reported in this work are based on a network model of the U.S. chemical manufacturing industry[11] which includes 873 chemical processes and 283 different chemicals, with stoichiometric and process utility data originally obtained from the IHS 2012 Process Economics Program Yearbook.[12] In 2019, the model was updated by DeRosa et al.[13] with the construction of a geographically resolved network. This geographically resolved model represents the U.S. petrochemical industry in 2017 and maps the interconnections of 249 chemical processes that produce hundreds of commodity chemicals and intermediates. Locations of production facilities are spatially resolved and include production capacity information originally derived from the 2017 ICIS Supply and Demand Database.[14] A total of 135 processes, with information from both the network and geographically resolved models, are examined in this work. Details of the 135 processes included in this work are documented in the Supporting Information. Since the emission estimates are process-based, the productions of the same chemicals manufactured using different processes or feedstocks are assessed separately.

System Boundary. Figure 1 shows the system boundaries of greenhouse gas emission estimates of chemical manufacturing

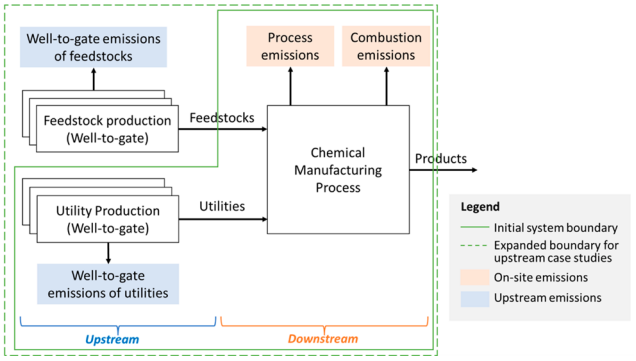

Figure 1. System boundaries of greenhouse gas emission estimates.

processes. Feedstocks and utilities (including natural gas, fuel oil, and electricity) produced and processed in upstream production are fed into downstream chemical manufacturing processes. As the chemical manufacturing industry is highly networked with products and coproducts from some processes used as feedstocks for other processes, the well-to-gate emission estimates of feedstocks can be very complicated and are excluded from the initial system boundary. The initial system boundary, including on-site emissions from chemical manufacturing processes and well-to-gate emissions of utilities, is designed to highlight emissions associated with downstream processes and is applied to the majority of processes estimated in this work. To evaluate the impacts of upstream sourcing and allocation choices on life cycle emission estimates of selected downstream chemicals, an expanded boundary adding well-to-gate emissions of feedstocks was applied. Greenhouse gas emissions associated with materials other than feedstocks and utilities (e.g., catalysts, makeup solvents) are beyond the system boundaries of this work. Greenhouse gases included in the analyses are methane, carbon dioxide, and nitrous oxide.

Sources of Emissions Associated with Downstream Processes (Initial System Boundary). Greenhouse gas emissions associated with each of the 135 processes are estimated based on process stoichiometry and utility usage data originally from the IHS 2012 Process Economics Program Yearbook and capacity data derived from the 2017 ICIS Supply and Demand Database. We assume the process stoichiometry and utility usage do not change significantly after the plants are built.[12−14] Both on-site emissions of the chemical manufacturing processes and upstream emissions of the utility sources are estimated. On-site emissions (gate-to-gate emissions) include combustion emissions and process emissions. Combustion emissions occur due to process utility usage, such as emissions from the combustion of natural gas and fuel oil (e.g., in boilers). Combustion processes of these two fuels were tracked separately. Accounting for steam generation and usage in chemical manufacturing operations is difficult. Because chemical manufacturing processes are frequently in large facilities and colocated with multiple processes, steam generation and usage is generally integrated across multiple processes, and so no emissions or credits were assigned to steam usage or generation in this work. Process emissions are usually from the chemical reactions that are involved in the production of the desired product. For example, the CO_2 produced from the water−gas shift reaction involved in the production of ammonia from natural gas via steam reforming, if not captured or utilized, will be emitted to the atmosphere as process

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emissions. The mass ratio of process CO_2 emissions to the ammonia product, without carbon capture, is approximately 1:1.[2]

Upstream emissions of the utility sources are associated with the production of utilities. For example, if natural gas is combusted for process heat, emissions associated with upstream oil and gas production assigned to the natural gas product are considered as upstream emissions for the natural gas combusted. Similarly, if electricity is used as a process utility, well-to-gate emissions associated with electricity source production and electricity generation are considered as upstream emissions for the electricity used. Total emissions associated with utility sources are the sum of upstream emissions of the utility sources and combustion emissions on-site. Combustion emissions of these energy sources are usually more significant compared to the upstream emissions; however, for processes relying on electricity sources, upstream emissions can significantly impact the emission profile of the process. In addition, if a fuel is sourced from a high emission fuel production region, upstream emissions can become significant.

National average emission factors for the utility sources, used in base case calculations, are derived from the GREET 2020 model and summarized in Table 1.[9] Electricity is assumed to be generated from a mix of sources including natural gas (33%), coal (29%), nuclear power (20%), residual oil (<1%), biomass (<1%), and others (16%), reported as U.S. Mix in GREET 2020. Greenhouse gas emissions are reported as carbon dioxide equivalents (CO_2e) with methane emissions assigned a carbon dioxide equivalent of 30 kg CO_2e per kg methane and N_2O emissions assigned a carbon dioxide equivalent of 265 kg CO_2e emissions per kg, based on 100-year GWPs. Recognizing many chemical manufacturing processes produce multiple products, the purpose of these analyses is to map process-based emission intensities across the chemical manufacturing industry. Therefore, all emissions are reported per process and quantified as emissions per unit mass of the primary product and emissions per process per year, multiplying the emissions per unit mass of the primary product by the production capacity of the primary product in the United States. No allocation methods are involved at this stage of analysis.

Table 1. Upstream and Combustion Emission Factors for Fuel and Electricity Uses Based on National Average Values

emission types	natural gas	fuel oil	electricity
upstream emissions (upstream of chemical facility) g CO_2e/MJ	11	4.6	125
combustion emissions (on-site) g CO_2e/MJ	56	81	0
total emissions g CO_2e/MJ	67	86	125

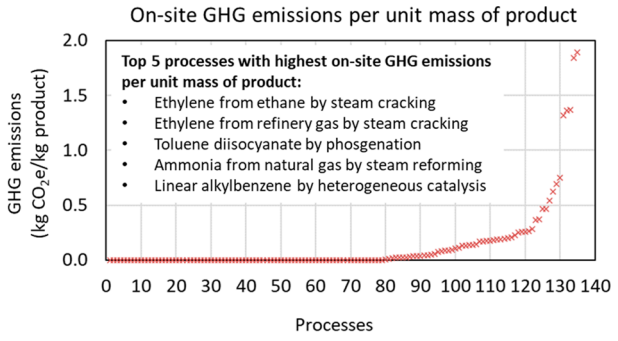
Upstream Sourcing and Allocation Case Studies (Expanded System Boundary). Data from the Eagle Ford Shale[14,15] are used to illustrate the impacts of different allocation and quantification methods for greenhouse gas emissions (both carbon dioxide and methane) from upstream oil and gas production on the life cycle (well-to-gate) greenhouse gas emissions of two downstream processes. The two processes selected in case studies are ethylene production from natural gas liquids (primarily ethane) via steam cracking and ammonia production from natural gas via steam methane reforming. Emissions from these processes are normalized by the production rate of the primary product (ethylene or ammonia); no credits are taken for the production of coproducts. Life cycle emissions of ethylene and ammonia products include emissions within the initial system boundary in Figure 1 and emissions from upstream production of natural gas and natural gas liquid feedstocks.

Three upstream emission quantification and allocation scenarios for oil and gas feedstocks are examined. In the base case scenario, greenhouse gas emissions in production, gathering, and gas processing operations are assigned to multiple products generated at these stages, based on the energy content of the product streams, and methane emissions are quantified with 100-year GWP. The second scenario applies the same allocation procedure for upstream emissions, but a 20-year GWP is applied for methane. The third scenario assumes all of the upstream emissions in the original assessment are assigned to the natural gas product, with a 20-year GWP applied for methane. These three scenarios were chosen to represent long-term and near-term horizons in climate reporting and the literature that has emerged for evaluating natural gas. The 100-year GWP and 20-GWP represent long-term and near-term greenhouse gas impacts, respectively. In greenhouse gas emission reporting for natural gas systems, some literature reports emissions using energy-based allocations, but more often, methane emissions are reported as methane emission intensity, generally defined as methane emissions divided by methane production or natural gas production, which simply assign methane emissions entirely to natural gas.[8] These allocation choices have more significant impacts on emission estimates in regions with comparable amounts of oil and gas products.[15]

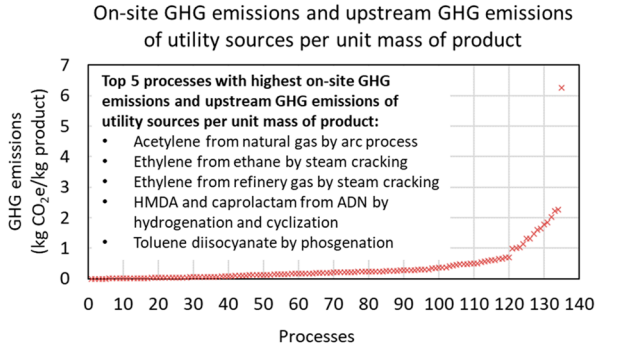
The Eagle Ford Shale is broadly representative of a wide range of production characteristics, with dry gas production regions, wet gas (gas and condensate) production regions, and oil production regions. Greenhouse gas emissions in the Eagle Ford Shale exhibit significant spatial variability ranging from 3 to 14 g CO_2E/MJ (with 100-year GWPs applied) between oil rich and gas rich regions.[15−17] In the analysis presented here, natural gas and natural gas liquids feedstocks for the selected downstream processes are assumed to be sourced from oil and gas production regions with different emission profiles in the Eagle Ford.

RESULTS AND DISCUSSION

Greenhouse Gas Emissions of Chemical Manufacturing Processes. Figure 2a shows on-site greenhouse gas emissions per kg of primary product, and Figure 2b shows greenhouse gas emissions including upstream emissions associated with the provision of process energy inputs per kilogram of product, for the 135 processes that are evaluated. The five most greenhouse gas-intensive processes, based on on-site combustion and process emissions, are ethylene from



(a)



(b)

Figure 2. Greenhouse gas emissions per unit mass of primary product.

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ethane by steam cracking, ethylene from refinery gas by steam cracking, toluene diisocyanate (TDI) by phosgenation, ammonia from natural gas by steam methane reforming, and linear alkyl benzene by heterogeneous catalysis. When upstream emissions of utilities are included, acetylene from natural gas by the arc process, with the highest electricity demand among all the processes evaluated, becomes the process with highest emission intensity. This is followed by the two ethylene production processes, hexamethylenediamine (HMDA, coproduct) and caprolactam (main product) from adiponitrile (ADN) by hydrogenation and cyclization and the TDI production described above. In both cases, with and without upstream emissions associated with process utilities, ethylene production via steam cracking and TDI production via phosgenation are among the processes with the highest emissions estimated per unit mass of product in the U.S. petrochemical industry. Only counting on-site combustion and process emissions overlooks the associated burdens of consuming electricity in the processes and the differences in upstream burdens of process fuels. Therefore, the following analyses will focus on the assessments with both on-site and upstream emissions of the utility sources.

In Figure 2b, some of the greenhouse gas intensive processes produce relatively small volumes of products, while others are high-volume, such as those that produce ethylene, ammonia, and chlorine. Figure 3 shows the emissions per unit mass of product multiplied by production capacity, with the horizontal axis representing greenhouse gas emissions per process per year in ascending order, and vertical axes representing cumulative emissions and cumulative percentage of total emissions from all the processes evaluated. A small number of processes dominate the total greenhouse gas emissions in the U.S. petrochemical industry. Ethylene, ammonia, and chlorine production contribute approximately 70% of total greenhouse gas emissions of the 135 chemical processes evaluated, and ethylene production alone contributes approximately half of total greenhouse gas emissions. Emission profiles of all 135 processes evaluated are documented in the Supporting Information.

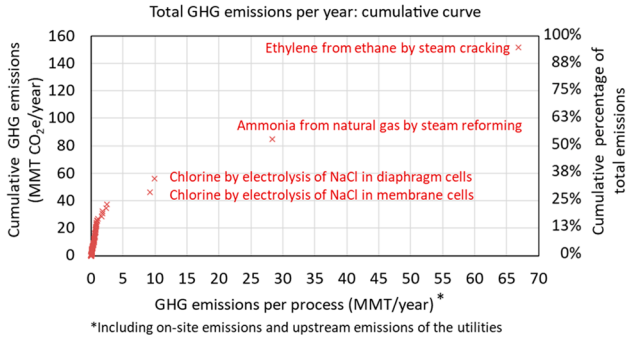

Figure 3. Greenhouse gas emissions per unit mass of product multiplied by U.S. production capacity in 2017.

Case Studies on Upstream Sourcing and Allocations. The well-to-gate greenhouse gas emissions of ethylene (from ethane) and ammonia production are evaluated, with different upstream emission allocation and quantification scenarios. The emissions associated with the oil and gas feedstocks are estimated based on three categories of production regions in the Eagle Ford Shale, including oil with associated gas production regions, wet gas production regions, and dry gas production regions. Chen et al. identified significant spatial variability in greenhouse gas emissions across the Eagle Ford Shale, due to differences in geographical characteristics, operation conditions, and emission control strategies.[15] Table 2 shows production basin greenhouse gas emissions of natural gas, natural gas liquids, and condensate oil with three different upstream emission allocation and quantification scenarios.[8,15] Emission burdens of the natural gas feedstocks vary by over 10-fold depending on how upstream emissions are sourced and allocated. Assigning all upstream emissions to natural gas only leads to burden-free natural gas liquids and oil feedstocks.

The differences in emission estimates of feedstock sources lead to significant differences in life cycle emission estimates of the downstream chemicals. Table 3 shows life cycle greenhouse gas emission estimates of ethylene (from ethane) and ammonia production with different upstream emission allocation and quantification scenarios, by combining the emission estimates for upstream feedstock production based in the Eagle Ford Shale and estimates of downstream chemical manufacturing described above. Life cycle emissions of ethylene production vary from 2.5 to 4.2 kg CO_2e/kg ethylene, and life cycle emissions of ammonia production vary from 1.6 to 2.9 kg CO_2e/kg ammonia.

For the products produced from natural gas liquids and condensate oil (e.g., ethylene), the assignment of all upstream emissions to natural gas results in a decrease in life cycle greenhouse gas emissions compared to an assessment assigning the emissions to multiple products. For example, if all of the upstream greenhouse gas emissions are assigned to natural gas, then none of the emissions should be assigned to natural gas liquids or oil coproduced with the gas. For polyethylene, if all of the upstream greenhouse gas emissions are assigned to natural gas, none should be assigned to the production of the ethane used to make the polyethylene. In this case, efforts to encourage plastics recycling for greater circularity (e.g., the circular footprint formula[18]) will identify a lower greenhouse gas benefit from recycling, which could adversely affect efforts to reduce plastic waste. For other products produced from natural gas (e.g., ammonia and hydrogen), assigning all of the upstream emissions to natural gas will increase life cycle greenhouse gas emissions compared to an energy based allocation.

The results in Tables 2 and 3 demonstrate that differences in how greenhouse gas emissions from oil and gas production, dominated by methane emissions, are allocated and quantified can have a range of effects on life cycle greenhouse gas emissions of downstream chemicals. However, if the source of the hydrocarbons is a production region that generates only one product (e.g., a dry gas region producing only natural gas), the effect is negligible. If the source of hydrocarbons is a production region that generates multiple products (e.g., an oil production region with associated gas), the effect is significant. In the United States, both types of production operations produce large quantities of gas. The effects can be even more significant if the source of hydrocarbons is a production region with high emission intensities. Sensitivity analyses are done in Table 4 with tripled upstream emission intensities of the wet gas regions in the Eagle Ford Shale, to represent the scenarios in regions with high emission intensities (e.g., the Permian Basin in west Texas).

Uncertainties. Uncertainties in the above estimates are mainly due to the assumptions made for utilities. As stated in

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Table 2. Life Cycle Greenhouse Gas Emissions of Natural Gas, Natural Gas Liquids, and Condensate Oil with Different Upstream Emission Allocation and Quantification Scenarios[8,15]

emission units: g CO_2e/MJ energy production	greenhouse gas intensity using 100-year global warming potentials and with upstream emissions assigned to multiple products	greenhouse gas intensity using 20-year global warming potentials and with upstream emissions assigned to multiple products	revised greenhouse gas intensity using 20-year global warming potentials and with all upstream emissions assigned to natural gas
associated natural gas[a]	4.3	7.9	58
natural gas from a wet gas region[b]	6.4	11	28
natural gas from a dry gas region[c]	13	22	25
natural gas liquids from an oil production region with associated gas[a]	4.3	7.9	0
natural gas liquids from a wet gas region[b]	6.4	11	0
natural gas liquids from a dry gas region[c]	13	22	0
condensate oil from an oil production region with associated gas[a]	4.3	7.9	0
condensate oil from a wet gas region[b]	6.4	11	0

[a]Oil with associated gas production regions in the northwest of the Eagle Ford Shale in Texas; emission intensities for upstream oil and gas production are averaged across Eagle Ford regions 1−5 in Chen et al.[15] [b]Wet gas production regions in the middle of the Eagle Ford Shale in Texas; emission intensities for upstream oil and gas production are averaged across Eagle Ford regions 6−11 in Chen et al.[15] [c]The dry gas region in the southeast of the Eagle Ford Shale in Texas; emission intensities for upstream oil and gas production in the Eagle Ford region 12 in Chen et al.[15] are applied.

Table 3. Life Cycle Greenhouse Gas Emission Estimates of Ethylene and Ammonia Production with Different Upstream Emission Allocation and Quantification Scenarios

emission units: kg CO_2e emissions/kg product	greenhouse gas intensity using 100-year global warming potentials and with upstream emissions assigned to multiple products	greenhouse gas intensity using 20-year global warming potentials and with upstream emissions assigned to multiple products	revised greenhouse gas intensity using 20-year global warming potentials and with all upstream emissions assigned to natural gas
ethylene produced from ethane from:			
(a) an oil region[a]	(a) 2.6	(a) 3.1	2.5 (same for all region scenarios as no upstream emissions are assigned to ethane feedstock)
(b) a wet gas region[b]	(b) 2.7	(b) 3.3	
(c) a dry gas region[c]	(c) 3.2	(c) 4.2	
Ammonia produced from natural gas from:			
(a) an oil region[a]	(a) 1.6	(a) 1.7	(a) 2.9
(b) a wet gas region[b]	(b) 1.6	(b) 1.8	(b) 2.2
(c) a dry gas region[c]	(c) 1.8	(c) 2.1	(c) 2.1

[a]Oil with associated gas production regions in the northwest of the Eagle Ford Shale in Texas; emission intensities for upstream oil and gas production are averaged across Eagle Ford regions 1−5 in Chen et al.[15] [b]Wet gas production regions in the middle of the Eagle Ford Shale in Texas; emission intensities for upstream oil and gas production are averaged across Eagle Ford regions 6−11 in Chen et al.[15] [c]The dry gas region in the southeast of the Eagle Ford Shale in Texas; emission intensities for upstream oil and gas production in the Eagle Ford region 12 in Chen et al.[15] are applied.

Table 4. Life Cycle Greenhouse Gas Emission Estimates of Ethylene and Ammonia Production with Different Upstream Emission Allocation and Quantification Scenarios, in a High Emission Intensity Oil and Gas Region with Tripled Emissions of the Wet Gas Regions in the Eagle Ford Shale

product	greenhouse gas intensity using 100-year global warming potentials and with upstream emissions assigned to multiple products	greenhouse gas intensity using 20-year global warming potentials and with upstream emissions assigned to multiple products	revised greenhouse gas intensity using 20-year global warming potentials and with all upstream emissions assigned to natural gas
natural gas	19 g CO_2e/MJ	33 g CO_2e/MJ	84 g CO_2e/MJ
condensate oil	6.4 g CO_2e/MJ	33 g CO_2e/MJ	0
ethylene produced from ethane	3.6 kg CO_2e/kg ethylene	4.9 kg CO_2e/kg ethylene	2.5 kg CO_2e/kg ethylene
ammonia produced from natural gas	1.9 kg CO_2e/kg ammonia	2.3 kg CO_2e/kg ammonia	3.5 kg CO_2e/kg ammonia

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the Materials and Methods section, the emission factors for the utilities are based on national average estimates, without differentiating utility sources among different types of plants and in different regions. For example, electricity used in the above processes is assumed to be generated from a mix of natural gas and other energy sources. However, in regions with extensive wind power (e.g., west Texas), electricity is primarily generated from wind power, providing burden free electricity. On the other hand, in regions with extensive coal mines (e.g., West Virginia), electricity is primarily generated from coal. The processes that significantly rely on electricity (e.g., acetylene production via arc process) may have completely different emission profiles depending on the location of the manufacturing facility and local shares of electricity sources. Integrating the region-specific electricity use with the spatially resolved chemical manufacturing network will provide more accurate estimates of greenhouse gas emissions for individual processes.

Though the fuels combusted on site are assumed to be natural gas and/or fuel oil for above processes, other types of fuels (e.g., natural gas liquids) and different heating values and heating efficiencies can be expected. Emission factors for the fuels would vary significantly depending on from where the fuels are sourced. In addition, the emission burdens or credits associated with steam use and generation were not counted in this work, assuming steam comes from other processes in integrated facilities as a burden free utility. However, depending on how steam is generated, emission burdens associated with steam generations may also be considered.

Emissions estimated for chemical processes were reported as process-based emissions without allocating to products in this work. For standalone facilities without production of coproducts, the emission values reported for the process are identical to the emissions allocated to the product. However, chemical manufacturing processes are highly integrated, and a process may produce multiple products. In this case, allocation by mass or market value may be appropriate coproduct handling methods. Displacement (system expansion) is also a possibility but may not be appropriate for mature industries and products that are unlikely to be displacing chemical production elsewhere.

A next stage of this analysis could address these three sources of uncertainty and variation (spatial factors, heat integration, coproduct handling) present in this stage.

Implications. A wide range of policies and voluntary initiatives are in place or are currently being advanced that rely on quantifying life cycle greenhouse gas emissions of oil and gas products. These include low carbon fuel standards, renewable fuel standards, greenhouse gas emission labeling of natural gas, emissions trading schemes, and the Clean Development Mechanism for developing economies and emerging EU regulations. For these initiatives to consistently assess greenhouse gas emissions, clear guidance is needed on accepted methods for allocating emissions. In the absence of clear guidance, different emission allocation methods could lead to very different greenhouse gas emissions for the same product, and different allocation methods applied to different products (e.g., assigning all methane emissions to a natural gas product while assigning oil production emissions to gasoline based on a multiproduct, energy based allocation) could lead to double counting of emissions.

In addition, when assessing the emission burdens of downstream chemicals and identifying potential emission reduction opportunities, the wide variation in emissions from upstream production of feedstock sources should be taken into consideration. Different feedstock sourcing, emission allocation, and quantification methods could all lead to significantly different estimates of life cycle emissions of the downstream chemicals. Consistent and transparent metrics for upstream emission estimates is an important enabler of low carbon goals worldwide.

CONCLUSION

Greenhouse gas emissions from 135 commodity chemical manufacturing processes in the United States were estimated. A small number of processes, with both high emission intensities and high production volumes, dominated the total greenhouse gas emissions of the processes evaluated. Well-to-gate emission estimates were performed for ethylene and ammonia production, to demonstrate the effect of feedstock sourcing and upstream emission allocation and quantification methods for well to gate emission estimates of downstream chemicals. Depending on how upstream emissions are allocated among oil and gas feedstocks, well-to-gate emission estimates of ammonia (from natural gas via steam methane reforming) and ethylene (from ethane via steam cracking) ranged from 1.6 to 2.9 kg CO_2e/kg and from 2.5 to 4.2 kg CO_2e/kg production, respectively. Accurately characterizing emissions from upstream production of feedstock sources with consistent and transparent allocation and quantification metrics is important in identifying decarbonization potentials for chemical manufacturing.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.2c00295.

On-site combustion and process emissions associated with the 135 chemical manufacturing processes; on-site emissions and upstream emissions of utilities associated with the 135 chemical manufacturing processes; and on-site emissions and upstream emissions of utilities per mass of product multiplied by U.S. production capacity in 2017 for the 135 processes (PDF)

AUTHOR INFORMATION

Corresponding Author

David T. Allen − *Center for Energy and Environmental Resources, The University of Texas at Austin, Austin, Texas 78758, United States;* orcid.org/0000-0001-6646-8755; Email: allen@che.utexas.edu

Authors

Qining Chen − *Center for Energy and Environmental Resources, The University of Texas at Austin, Austin, Texas 78758, United States;* orcid.org/0000-0003-1690-8091

Jennifer B. Dunn − *Department of Chemical and Biological Engineering and Center for Engineering Sustainability and Resilience, Northwestern University, Evanston, Illinois 60208, United States;* orcid.org/0000-0002-2065-5106

Complete contact information is available at: https://pubs.acs.org/10.1021/acssuschemeng.2c00295

Notes

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