CRADLE-TO-RESIN LIFE CYCLE ANALYSIS OF POLYETHYLENE TEREPHTHALATE RESIN

Final Revised Report

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PREFACE

This life cycle assessment of polyethylene terephthalate (PET) resin was funded by the National Association for PET Container Resources (NAPCOR). The report was made possible through the cooperation of NAPCOR member companies, who provided data for the production of many of the intermediate chemicals and the final PET resin.

This report was prepared for NAPCOR by Franklin Associates, A Division of Eastern Research Group, Inc. as an independent contractor. This project was managed and primarily authored by Melissa Huff, Senior LCA Analyst and Project Manager. Anne Marie Molen assisted with data collection tasks, modeling, and report and appendix preparation. Mariya Absar aided with research, modeling and appendix preparation. Ben Young assisted with research.

Franklin Associates gratefully acknowledges the significant contribution to this project by Rick Moore of NAPCOR in leading this project. Also acknowledged are the following companies: BP, DAK Americas, Indorama Corporation, Nan Ya Plastics Corporation, Chevron Phillips Chemical Corporation, Huntsman Corporation, INEOS Olefins, and the Dow Chemical Company, who graciously provided primary Life Cycle Inventory data for the PET resin and many intermediate chemicals. Their effort in collecting data has added considerably to the quality of this LCA report.

Franklin Associates makes no statements other than those presented within the report.

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CRADLE-TO-GATE LIFE CYCLE ASSESSMENT OF POLYETHYLENE TEREPHTHALATE RESIN

INTRODUCTION

This study provides the National Association for PET Container Resources (NAPCOR), their members, users of the U.S. LCI Database, and the public at large with information about the life cycle inventory and impacts for average virgin polyethylene terephthalate (PET) resin used within a variety of products in North America. Life cycle assessment (LCA) is recognized as a scientific method for making comprehensive, quantified evaluations of the environmental benefits and tradeoffs commonly for the entire life cycle of a product system, beginning with raw material extraction and continuing through disposition at the end of its useful life as shown in Figure 1 below. This cradle-to-gate LCA includes the life cycle stages shown in the dashed box including the "Raw Materials Acquisition" and "Materials Manufacture" boxes in the figure.

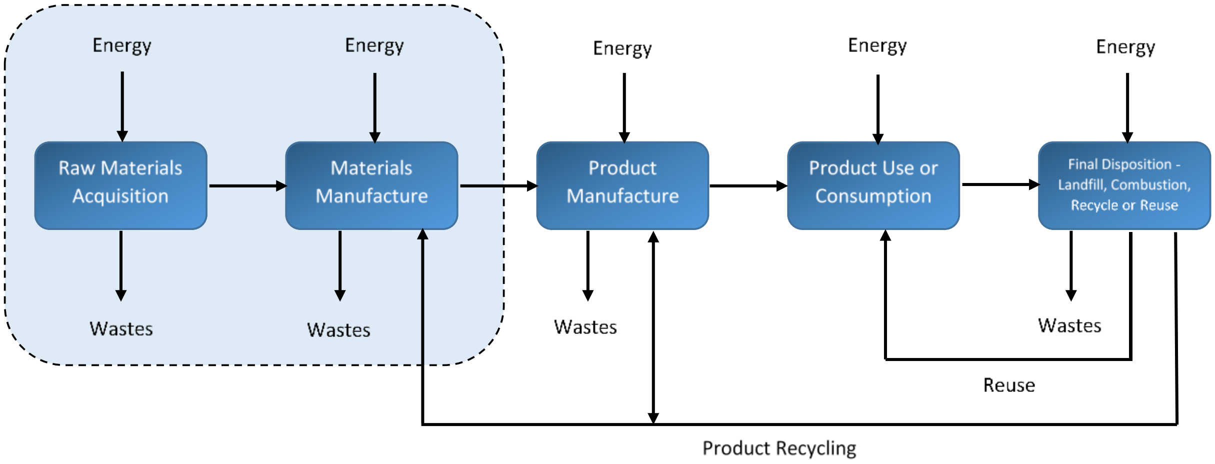

Figure 1. General materials flow for "cradle-to-grave" analysis of a product system. The dashed box indicates the boundaries of this analysis.

The results of this analysis are useful for understanding production-related impacts and are provided in a manner suitable for incorporation into full life cycle assessment studies. The information from an LCA can be used as the basis for further study of the potential improvement of resource use and environmental impacts associated with product systems. It can also pinpoint areas (e.g., material components or processes) where changes would be most beneficial in terms of reducing energy use or potential impacts.

A life cycle assessment commonly examines the sequence of steps in the life cycle of a product system, beginning with raw material extraction and continuing through material production, product fabrication, use, reuse or recycling where applicable, and final disposition. This cradle-to-gate life cycle inventory (LCI) and life cycle impact assessment

(LCIA) quantifies the total energy requirements, energy sources, water consumption, atmospheric pollutants, waterborne pollutants, and solid waste resulting from the production of polyethylene terephthalate resin. It is considered a cradle-to-gate boundary system because this analysis ends at the resin production. The system boundaries stop at resin production so that the resin data can be linked with fabrication, use, and end-of-life data to create full life cycle inventories for a variety of PET products, such as automotive parts or packaging. The method used for this inventory has been conducted following internationally accepted standards for LCI and LCA methodology as outlined in the ISO 14040 and 14044 standard documents[1].

This LCA boundary ends at material production. An LCA consists of four phases:

- Goal and scope definition
- Life cycle inventory (LCI)
- Life cycle impact assessment (LCIA)
- Interpretation of results

The LCI identifies and quantifies the material inputs, energy consumption, water consumption, and environmental emissions (atmospheric emissions, waterborne wastes, and solid wastes) over the defined scope of the study. The LCI data for this analysis of PET resin is shown separately as unit processes in the attached Appendix. Those unit processes that have been updated will be made available to the National Renewable Energy Laboratory (NREL) who maintains the U.S. LCI Database.

In the LCIA phase, the inventory of emissions is classified into categories in which the emissions may contribute to impacts on human health or the environment. Within each impact category, the emissions are then normalized to a common reporting basis, using characterization factors that express the impact of each substance relative to a reference substance.

STUDY GOAL AND SCOPE

In this section, the goal and scope of the study is defined, including information on data sources used and methodology.

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[1] International Standards Organization. ISO 14040:2006 Environmental management—Life cycle assessment—Principles and framework, ISO 14044:2006, Environmental management – Life cycle assessment – Requirements and guidelines.

STUDY GOAL AND INTENDED USE

The purpose of this LCA is to document the LCI data and then evaluate the environmental profiles of polyethylene terephthalate resin. The intended use of the study results is twofold:

- To provide the LCA community and other interested parties with average North American LCI data for PET resin, and
- to provide information about the environmental burdens associated with the production of PET resin. The LCA results for the PET resin system can be used as a benchmark for evaluating future updated PET resin results for North America.

According to ISO 14040 and 14044 standards, a peer review is not required as no comparative assertions of competing materials or products are made in this study. This LCA compares the current results with similar PET resins results previously published by ACC Plastics Division in 2011.

This report is the property of NAPCOR and may be used by the trade association or members or the general public at NAPCOR's discretion.

FUNCTIONAL UNIT

The function of PET resin is its ability to be used in a variety of PET products, for example, bottles and automotive products. As the study boundary concludes at material manufacture, a mass functional unit has been chosen. Results for this analysis are shown on a basis of both a 1,000 pounds and a 1,000 kilograms of PET resin.

SCOPE AND BOUNDARIES

This LCA quantifies energy and resource use, water consumption, solid waste, and environmental impacts for the following steps in the life cycle of the PET resin produced from purified terephthalic acid (PTA):

- Raw material extraction (e.g., extraction of petroleum and natural gas as feedstocks for plastic resin), and intermediate material processing, including incoming transportation for each process through PTA production,
- Raw material extraction (e.g., extraction of petroleum and natural gas as feedstocks for plastic resin), and intermediate material processing, including incoming transportation for each process through ethylene glycol (EG) production, and
- PET resin manufacture, including incoming electricity, fuels, metals mining/processing used to create catalysts for PET, and transportation for each material.

PET produced from dimethyl terephthalate (DMT) has not been included in this analysis. Some PET is produced from DMT in North America; however, the amount of PET is small, and the resin is used for a limited number of specialized products.

This report presents LCI results, as well as LCIA results, for the production of PET resin split out by cradle-to-PTA production, cradle-to-EG production, and PET production as described previously in this section. Figure 2 presents the flow diagram for the production of PET resin. Process descriptions and individual process tables for each box shown in the flow diagram can be found in the attached appendix.

The following are not included in the study:

- **Miscellaneous materials and additives.** Selected materials such as catalysts, pigments, ancillary materials, or other additives which total less than one percent by weight of the net process inputs are typically not included in assessments. Omitting miscellaneous materials and additives keeps the scope of the study focused. It is possible that production of some substances used in small amounts may be energy and resource intensive or may release toxic emissions; however, the impacts would have to be very large in proportion to their mass in order to significantly affect overall results and conclusions. For this study, the use of metals (e.g. antimony, cobalt, titanium) to create catalysts used in PET manufacture does affect the eutrophication results and so the mining/processing step has been included in this case; however, the production of the catalyst itself is excluded. With the exception of the metals used for creating the catalysts used in the manufacture of PET, the results for the resin are not expected to be understated by any significant amount due to substances that may be used in small amounts.
- **Capital equipment, facilities, and infrastructure.** The energy and wastes associated with the manufacture of buildings, roads, pipelines, motor vehicles, industrial machinery, etc. are not included. The energy and emissions associated with production of capital equipment, facilities, and infrastructure generally become negligible when averaged over the total output of product or service provided over their useful lifetimes.
- **Space conditioning.** The fuels and power consumed to heat, cool, and light manufacturing establishments are omitted from the calculations when possible. For manufacturing plants that carry out thermal processing or otherwise consume large amounts of energy, space conditioning energy is quite low compared to process energy. The data collection forms developed for this project specifically requested that the data provider either exclude energy use for space conditioning or indicate if the reported energy requirements included space conditioning. Energy use for space conditioning, lighting, and other overhead activities is not expected to make a significant contribution to total energy use for the resin system.
- **Support personnel requirements**. The energy and wastes associated with research and development, sales, and administrative personnel or related activities have not been included in this study. Similar to space conditioning, energy requirements and related emissions are assumed to be quite small for support personnel activities.

The geographic scope of the analysis is the manufacture of PET resin in North America. The majority of the data used in the modeling is from North American databases (U.S. LCI database, Franklin Associates' private database). In cases where it was necessary to use supplemental data from a European database, the data sets were adapted to the extent possible to represent North American inputs and practices.

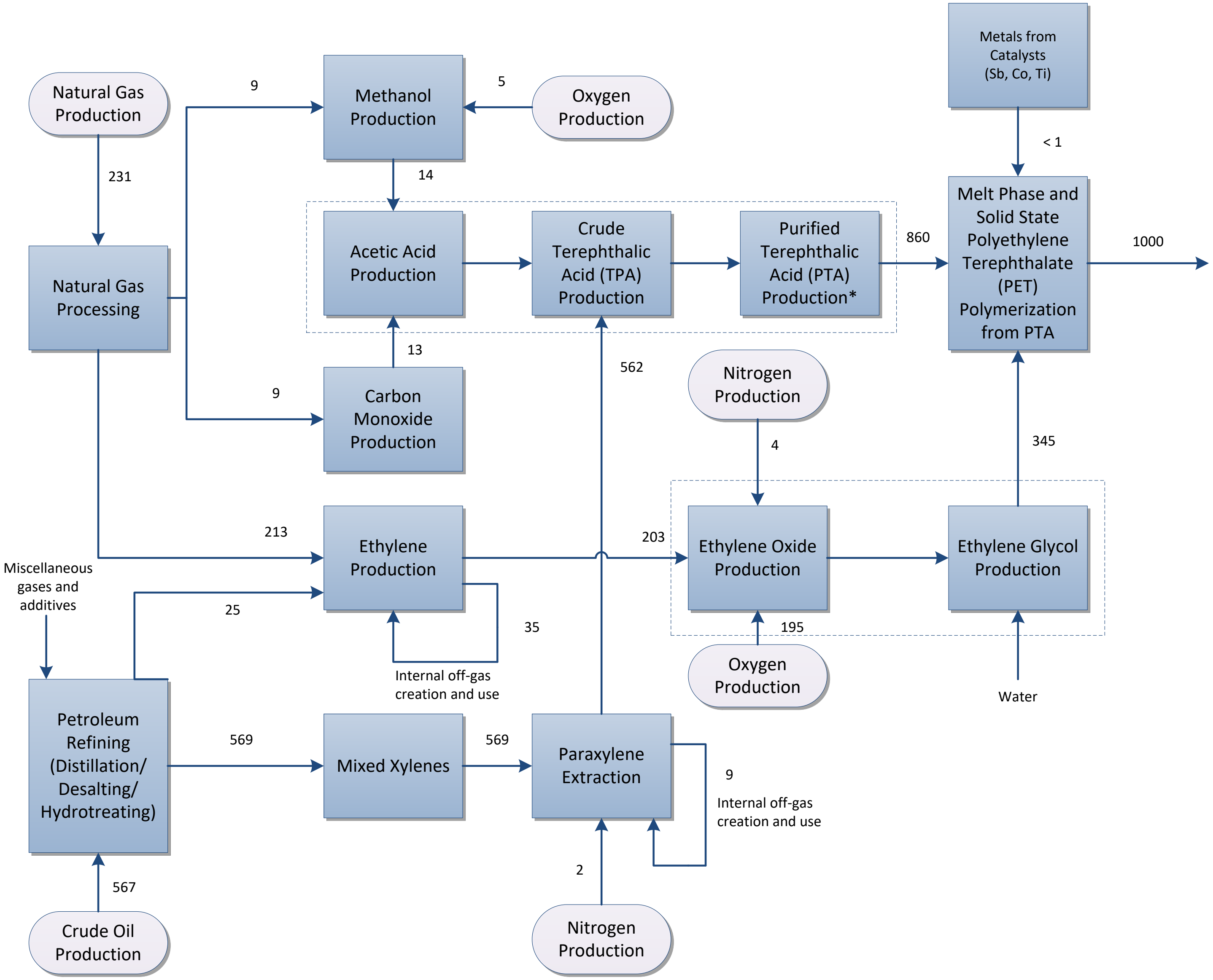

Figure 2. Flow diagram for the production of polyethylene terephthalate (PET) resin. Dotted rectangles represent aggregated datasets.

INVENTORY AND IMPACT ASSESSMENT RESULTS CATEGORIES

The full inventory of emissions generated in an LCA study is lengthy and diverse, making it difficult to interpret emissions profiles in a concise and meaningful manner. LCIAs helps to interpret of the emissions inventory. LCIA is defined in ISO 14044 Section 3.4 as the "phase of life cycle assessment aimed at understanding and evaluating the magnitude and significance of the potential environmental impacts for a product system throughout the life cycle of the product." In the LCIA phase, the inventory of emissions is first classified into categories in which the emissions may contribute to impacts on human health or the environment. Within each impact category, the emissions are then normalized to a common reporting basis, using characterization factors that express the impact of each substance relative to a reference substance.

The LCI and LCIA results categories and methods applied in this study are displayed in Table 1. This study addresses global, regional, and local impact categories. For most of the impact categories examined, the TRACI 2.1 method, developed by the United States Environmental Protection Agency (EPA) specific to U.S. conditions and updated in 2012, is employed.[2] For the category of Global Warming Potential (GWP), contributing elementary flows are characterized using factors reported by the Intergovernmental Panel on Climate Change (IPCC) in 2013 with a 100 year time horizon.[3] In addition, the following LCI results are included in the results reported in the analysis:

- Energy demand: this method is a cumulative inventory of all forms of energy used for processing energy, transportation energy, and feedstock energy. This analysis reports both total energy demand and non-renewable energy demand. Renewable and non-renewable energy demand are reported separately to assess consumption of fuel resources that can be depleted, while total energy demand is used as an indicator of overall consumption of resources with energy value. Energy is also categorized by individual fuel types, as well as by process/fuel vs. feedstock energy.
- Total solid waste is assessed as a sum of the inventory values associated with this category. This category is also broken into hazardous and non-hazardous wastes and their end-of-life (e.g. incineration, waste-to-energy, or landfill).
- Water consumption is assessed as a sum of the inventory values associated with this category and does not include any assessment of water scarcity issues.

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[2] Bare, J. C. Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI), Version 2.1 - User's Manual; EPA/600/R-12/554 2012.

[3] IPCC, 2013: *Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change* [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 2013.

Table 1. Summary of LCI/LCIA Impact Categories

	Impact/Inventory Category	Description	Unit	LCIA/LCI Methodology
LCI Categories	Total energy demand	Measures the total energy from point of extraction; results include both renewable and non-renewable energy sources.	MM Btu/MJ	Cumulative energy inventory
	Non-renewable energy demand	Measures the fossil and nuclear energy from point of extraction.	MM Btu/MJ	Cumulative energy inventory
	Renewable energy demand	Measures the hydropower, solar, wind, and other renewables, including landfill gas use.	MM Btu/MJ	Cumulative energy inventory
	Solid waste by weight	Measures quantity of fuel and process waste to a specific fate (e.g., landfill, WTE) for final disposal on a mass basis	Lb/kg	Cumulative solid waste inventory
	Water consumption	Freshwater withdrawals which are evaporated, incorporated into products and waste, transferred to different watersheds, or disposed into the land or sea after usage	Gallons/Liters	Cumulative water consumption inventory
LCIA Categories	Global warming potential	Represents the heat trapping capacity of the greenhouse gases. Important emissions: CO_2 fossil, CH_4, N_2O	Lb/kg CO_2 equivalents (eq)	IPCC (2013) GWP 100a*
	Acidification potential	Quantifies the acidifying effect of substances on their environment. Important emissions: SO_2, NO_x, NH_3, HCl, HF, H_2S	Lb/kg SO_2 eq	TRACI v2.1
	Eutrophication potential	Assesses impacts from excessive load of macro-nutrients to the environment. Important emissions: NH_3, NO_x, COD and BOD, N and P compounds	Lb/kg N eq	TRACI v2.1
	Ozone depletion potential	Measures stratospheric ozone depletion. Important emissions: CFC compounds and halons	Lb/kg CFC-11 eq	TRACI v2.1
	Smog formation potential	Determines the formation of reactive substances (e.g. tropospheric ozone) that cause harm to human health and vegetation. Important emissions: NO_x, BTEX, NMVOC, CH_4, C_2H_6,	Lb/kg O_3 eq	TRACI v2.1

	Impact/Inventory Category	Description	Unit	LCIA/LCI Methodology
		C_4H_{10}, C_3H_8, C_6H_{14}, acetylene, Et-OH, formaldehyde		

DATA SOURCES

The purpose of this study is to develop a life cycle profile for PET resin using the most recent data available for each process. A weighted average was calculated for all primary data collected for this analysis. Primary data has been collected for ethylene, paraxylene, ethylene oxide/ethylene glycol, crude terephthalic acid (TPA)/purified terephthalic acid (PTA) and PET resin production for the year 2015. Secondary data was researched and updated for methanol and mixed xylenes production in 2017 for this study. Updated secondary data was also researched in 2017 for crude oil extraction and refining and natural gas production and processing as part of the soon-to-be released update to the U.S. LCI plastics database commissioned by ACC Plastics Division. All other processes shown in Figure 2 used data from the previous PET dataset from 2005.

LCI data for the production of PET resin were collected from three producers (seven plants) in North America – all in the United States. All companies provided data for the year 2015. The captured production amount is approximately 50 percent[4] of the available capacity for all PET resin production in North America in 2015. Small amounts (less than 1 percent of total output) of off-spec/trim/scrap resin are produced as coproducts during this process. A mass basis was used to allocate the credit for the coproduct.

LCI data for the production of TPA/PTA was collected from three producers (three plants) in North America – all in the United States. Not all plants were able to provide data for 2015. One plant provided 2013 data and one provided 2016 data. These variances were due to plant issues (e.g. shut downs/updates/temporary maintenance shut downs) during 2015 that may have skewed the average. Small amounts (less than 1 percent of total output) of off-spec PTA are produced as coproducts during this process. A mass basis was used to allocate the credit for the coproduct.

LCI data for the production of ethylene oxide (EO)/ethylene glycol (EG) was collected from three producers (five EO plants/three EG plants) in North America – all in the United States. All plants were able to provide data for 2015 with the exception of emissions from one plant, which were from 2016 due to availability issues. Monoethylene glycol and Diethylene glycol were considered the main products; triethylene glycol, when produced, was considered a coproduct. A mass basis was used to allocate the credit for the coproduct.

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[4] Plastics Insight, 2016. *Global PET Resin Production Capacity.* October 12, 2016 Available at: https://www.plasticsinsight.com/global-pet-resin-production-capacity/ Calculations performed by Franklin Associates.

LCI data for the production of Paraxylene (PX) was collected from three producers (3 plants) in North America – all in the United States. Not all plants were able to provide data for 2015. One plant provided 2013 data and one provided 2016 data. These variances were due to plant issues (e.g. shut downs/updates/temporary maintenance shut downs) during 2015 that may have skewed the average. Coproducts include a number of aromatics, carbon dioxide, and some fuels. For the coproducts sold for material use in other processes, mass basis was used to allocate the credit for the coproduct. For coproducts sold for fuel use in other processes, these were treated as an avoided fuel product and were given credits based on the fuel they would replace.

LCI data for the production of olefins, including ethylene, were collected from three producers (ten plants) in North America – all in the United States. All companies provided data for the year 2015. A weighted average was calculated from the data collected and used to develop the LCA model. Propylene, pyrolysis gasoline and butadiene are among the coproducts of ethylene production, and a mass basis was used to allocate the credit for the coproducts. For coproducts sold for fuel use in other processes, these were treated as an avoided fuel product and were given credits based on the fuel they would replace.

The remaining raw material and intermediate materials used to produce PET resin are from secondary sources. All process descriptions and LCI data for unit processes are provided in the Appendix at the end of this report.

DATA QUALITY ASSESSMENT

ISO 14044:2006 lists a number of data quality requirements that should be addressed for studies intended for use in public comparative assertions. The data quality goals for this analysis were to use data that are (1) geographically representative for the PET resin based on the locations where material sourcing and production take place, and (2) representative of current industry practices in these regions. As described in the previous section, three companies each provided current, geographically representative data for all primary data collected for this LCA.

The remaining datasets were either updated using geographical and technologically relevant data from government or privately available statistics/studies within the US or drawn from either the U.S. LCI database or Ecoinvent[5]. The data sets used were the most current and most geographically and technologically relevant data sets available during the data collection phase of the project.

Consistency, Completeness, Precision: Data evaluation procedures and criteria were applied consistently to all primary data provided by the participating producers for all data

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[5] Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., and Weidema, B., 2016. The ecoinvent database version 3 (part I): overview and methodology. The International Journal of Life Cycle Assessment, [online] 21(9), pp.1218–1230. Available at: <http://link.springer.com/10.1007/s11367-016-1087-8> [Accessed Sept, 2018].

collected. All primary data obtained specifically for this study were considered the most representative available for the systems studied. Data sets were reviewed for completeness and material balances, and follow-up was conducted as needed to resolve any questions about the input and output flows, process technology, etc. The aggregated averaged datasets were also reviewed by the providing companies as compared to the provided dataset. Companies were requested to review whether their data were complete and to comment about their or the average dataset.

Reproducibility: To maximize transparency and reproducibility, the report identifies specific data sources, assumptions, and approaches used in the analysis to the extent possible; however, reproducibility of study results is limited to some extent by the need to protect certain data sets that were judged to be high quality and representative data sets for modeling purposes but could not be shown due to confidentiality.

Uncertainty: Uncertainty issues and uncertainty thresholds applied in interpreting study results are described in the following section.

DATA ACCURACY AND UNCERTAINTY

In LCA studies with thousands of numeric data points used in the calculations, the accuracy of the data and how it affects conclusions is truly a complex subject, and one that does not lend itself to standard error analysis techniques. Techniques such as Monte Carlo analysis can be used to assess study uncertainty, but the greatest challenge is the lack of uncertainty data or probability distributions for key parameters, which are often only available as single point estimates. However, steps are taken to ensure the reliability of data and results, as previously described.

The accuracy of the environmental results depends on the accuracy of the numbers that are combined to arrive at that conclusion. For some processes, the data sets are based on actual plant data reported by plant personnel, while other data sets may be based on engineering estimates or secondary data sources. Primary data collected from actual facilities are considered the best available data for representing industry operations. In this study, primary data were used to model the reclaimer processes used to produce the recycled resins. All data received were carefully evaluated before compiling the production-weighted average data sets used to generate results. Supporting background data were drawn from credible, widely used databases including the US LCI database and Ecoinvent.

METHOD

The LCA has been conducted following internationally accepted standards for LCA as outlined in the ISO 14040 and 14044 standards, which provide guidance and requirements for conducting LCA studies. However, for some specific aspects of LCA, the ISO standards have some flexibility and allow for choices to be made. The following sections describe the approach to each issue used in this study. Many of these issues are specific to the intermediate chemicals used (e.g. ethylene from steam crackers).

Raw Materials Use for Internal Energy in Steam Crackers

Some of the raw material inputs to the steam cracker create gases that are combusted to provide energy for the steam cracker, decreasing the amount of purchased energy required for the reaction. Data providers listed this energy as fuel gas or offgas and, in many cases, supplied the heating value of this gas. Using this information, Franklin Associates calculated the amount of raw material combusted within the steam cracker to produce this utilized energy source.

This internally created energy is included in the analysis by including the production of the raw materials combusted to produce the energy as well as the energy amount attributed to the combustion of those raw materials. Unlike the raw materials that become part of the product output mass, no material feedstock energy is assigned to the raw materials inputs that are combusted within the process.

Coproduct Allocation

An important feature of life cycle inventories is that the quantification of inputs and outputs are related to a specific amount of useful output from a process. However, it is sometimes difficult or impossible to identify which inputs and outputs are associated with individual products of interest resulting from a single process (or process sequence) that produces multiple useful products. The practice of allocating inputs and outputs among multiple products from a process is often referred to as coproduct allocation or credit.

Co-product credit is done out of necessity when raw materials and emissions cannot be directly attributed to one of several product outputs from a system. It has long been recognized that the practice of giving co-product credit is less desirable than being able to identify which inputs lead to specific outputs. In this study, co-product allocations are necessary because of multiple useful outputs from some of the "upstream" chemical processes involved in producing the resins used to manufacture plastic.

Franklin Associates follows the guidelines for allocating co-product credit shown in the ISO 14044:2006 standard on life cycle assessment requirements and guidelines[6]. In this standard, the preferred hierarchy for handling allocation is (1) avoid allocation where possible, (2) allocate flows based on direct physical relationships to product outputs, (3) use some other relationship between elementary flows and product output. No single allocation method is suitable for every scenario. As described in ISO 14044 section 4.3.4.2, when allocation cannot be avoided, the preferred partitioning approach should reflect the underlying physical relationships between the different products or functions.

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[6] International Standards Organization. ISO 14044:2006, Environmental management – Life cycle assessment – Requirements and guidelines.

Material Coproducts

Some processes lend themselves to physical allocation because they have physical parameters that provide a good representation of the environmental burdens of each co-product. Examples of various allocation methods are mass, stoichiometric, elemental, reaction enthalpy, and economic allocation. Simple mass and enthalpy allocation have been chosen as the common forms of allocation in this analysis. However, these allocation methods were not chosen as a default choice but made on a case by case basis after due consideration of the chemistry and basis for production.

Material coproducts were created in all the intermediate chemical process steps collected for this analysis, as well as the PET production. The material coproducts from PET and PTA production were off-spec or scrap product that is sold at a lower price. The material coproducts for EO/EG, paraxylene, and ethylene were separate products produced during the process.

A portion of the inputs and outputs calculated for the coproducts were removed from the total inputs and outputs, so that the remaining inputs and outputs only represented the main product in each unit process. The ratio of the mass of the coproduct over the total mass output was removed from the total inputs and outputs of the process, and the remaining inputs and outputs are allocated over the material products (Equation 1).

$$[IO] \times \left(1 - \frac{M_{CP}}{M_{Total}}\right) = [IO]_{attributed\ to\ remaining\ \ products} \qquad \text{(Equation 1)}$$

where
IO = Input/Output Matrix to produce all products/coproducts
M_{CP} = Mass of Coproduct
M_{Total} = Mass of all Products and Coproducts

Energy Coproducts Exported from System Boundaries

Some of the unit processes produce energy either as a fuel coproduct or as steam created from the process that is sent to another plant for use. To the extent possible, system expansion to avoid allocation was used as the preferred approach in the ISO 14044:2006 standard. Fuels or steam exported from the boundaries of the system would replace purchased fuels for another process outside the system. System expansion credits were given for avoiding the energy-equivalent quantity of fuel production and combustion displaced by the exported coproduct energy.

Electricity Grid Fuel Profile

Electricity production and distribution systems in North America are interlinked. Users of electricity, in general, cannot specify the fuels used to produce their share of the electric power grid. Data for this analysis was collected from plants in the United States. The U.S.

average fuel consumption by electrical utilities was used for the electricity within this analysis. This electricity data set uses the eGRID 2016 database[7] as shown below.

Source	Coal	Oil	Natural Gas	Nuclear	Hydro-power	Biomass	Other*
Percentage (EPA, 2018)	30.40%	0.60%	33.80%	19.80%	6.40%	1.70%	7.30%

* includes wind, geothermal, other renewable & unknown

Electricity generated on-site at a manufacturing facility is represented in the process data by the fuels used to produce it. If a portion of on-site generated electricity is sold to the electricity grid, credits for sold on-site electricity are accounted for in the calculations for the fuel mix.

Electricity/Heat Cogeneration

Cogeneration is the use of steam for generation of both electricity and heat. The most common configuration is to generate high temperature steam in a cogeneration boiler and use that steam to generate electricity. The steam exiting the electricity turbines is then used as a process heat source for other operations. Significant energy savings occur because in a conventional operation, the steam exiting the electricity generation process is condensed, and the heat is dissipated to the environment.

For LCI purposes, the fuel consumed and the emissions generated by the cogeneration boiler need to be allocated to the two energy-consuming processes: electricity generation and subsequent process steam. An energy basis was used for allocation in this analysis.

In order to allocate fuel consumption and environmental emissions to both electricity and steam generation, the share of the two forms of energy (electrical and thermal) produced must be correlated to the quantity of fuel consumed by the boiler. Data on the quantity of fuel consumed and the associated environmental emissions from the combustion of the fuel, the amount of electricity generated, and the thermal output of the steam exiting electricity generation must be known in order to allocate fuel consumption and environmental emissions accordingly. These three types of data are discussed below.

1. **Fuels consumed and emissions generated by the boiler:** The majority of data providers for this study reported natural gas as the fuel used for cogeneration. According to 2012 industry statistics, natural gas accounted for 65 percent of industrial cogeneration, while coal and waste gases (LPG surrogate used) accounted for the largest portion of the remaining fuels used.

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[7] Online database found at: https://www.epa.gov/energy/emissions-generation-resource-integrated-database-egrid

2. **Kilowatt-Hours of Electricity Generated:** In this analysis, the data providers reported the kilowatt-hours of electricity from cogeneration. The Btu of fuel required for this electricity generation was calculated by multiplying the kilowatt-hours of electricity by 6,826 Btu/kWh (which utilizes a thermal to electrical conversion efficiency of 50 percent). This Btu value was then divided by the Btu value of fuel consumed in the cogeneration boiler to determine the electricity allocation factor.

3. **Thermal Output of Steam Exiting Electricity Generation:** In this analysis, the data providers stated the pounds and pressure of steam from cogeneration. The thermal output (in Btu) of this steam was calculated from enthalpy tables (in most cases steam ranged from 1,000 to 1,200 Btu/lb). An efficiency of 80 percent was used for the industrial boiler to calculate the amount of fuel used. This Btu value was then divided by the Btu value of fuel consumed in the cogeneration boiler to determine the steam allocation factor.

LIFE CYCLE INVENTORY AND IMPACT ASSESSMENT RESULTS

This section presents baseline results for the following LCI and LCIA results for both 1,000 pounds and 1,000 kilograms of PET resin studied:

Life cycle inventory results:
- Cumulative energy demand
- Non-renewable energy demand
- Renewable energy demand
- Total energy by fuel type
- Solid waste by weight
- Water consumption

Life cycle impact assessment results:
- Global warming potential
- Acidification potential
- Eutrophication potential
- Ozone depletion potential
- Smog formation potential

Throughout the results sections, the tables and figures break out system results into the following categories:

- Cradle-to-PTA production
- Cradle-to-EG production
- PET resin production

The phrase “cradle-to-“ is defined as including all of the raw and intermediate chemicals required for the production of the chemical stated in the term. The word “system” is also used to describe the raw and intermediate materials for a chemical (e.g. PTA system)

ENERGY DEMAND

Cumulative Energy Demand

Cumulative energy demand results include all renewable and non-renewable energy sources used for process and transportation energy, as well as material feedstock energy. Process energy includes direct use of fuels, including the use of fossil fuels, hydropower, nuclear, wind, solar, and other energy sources to generate electricity used by processes. Fuel energy is the energy necessary to create and transport the fuels to the processes. The feedstock energy is the energy content of the resources removed from nature and used as material feedstocks for the PET resin (e.g., the energy content of oil and gas used as material feedstocks).

The average total energy required to produce PET resin is 26.4 million Btu per 1,000 pounds of resin or 61.4 GJ per 1,000 kilograms of resin. Table 2 shows total energy demand for the life cycle of the PET resin. The resin production energy has been split out from the cradle-to-PTA energy and cradle-to-EG energy. Less than 10 percent of the total energy is required to produce the resin itself. Over 60 percent of the total energy is required to produce the PTA system, while approximately 28 percent is needed to produce the EG system.

Table 2. Total Energy Demand for PET Resin

	Basis: 1,000 pounds		
	Total Energy	**Non-Renewable Energy**	**Renewable Energy**
	MM Btu	***MM Btu***	***MM Btu***
Cradle-to-PTA	16.7	16.6	0.13
Cradle-to-EG	7.25	7.22	0.024
Resin Production	2.41	2.35	0.064
Total	**26.4**	**26.2**	**0.22**
	Basis: 1,000 kilograms		
	Total Energy	**Non-Renewable Energy**	**Renewable Energy**
	GJ	***GJ***	***GJ***
Cradle-to-PTA	38.9	38.6	0.30
Cradle-to-EG	16.9	16.8	0.057
PET Production	5.60	5.47	0.15
Total	**61.4**	**60.9**	**0.50**
	Percentage		
	Total Energy	**Non-Renewable Energy**	**Renewable Energy**
	%	***%***	***%***
Cradle-to-PTA	63.4%	62.9%	0.5%
Cradle-to-EG	27.5%	27.4%	0.1%
PET Production	9.1%	8.9%	0.2%
Total	**100%**	**99.2%**	**0.8%**

Non-renewable energy demand includes the use of fossil fuels (petroleum, natural gas, and coal) for process energy, transportation energy, and as material feedstocks (e.g., oil and gas used as feedstocks for plastics), as well as use of uranium to generate the share of nuclear energy in the average U.S. kWh. More than 99 percent of the total energy comes from non-renewable sources. The landfill gas used for process energy and electricity derived from renewable energy sources (primarily hydropower, as well as wind, solar, biomass, and other sources) comprise the renewable energy demand. Of the renewable energy (less than one percent of the total energy), over 99 percent comes from a split of hydropower and other renewable sources (geothermal, solar, etc.) from electricity production, with the remaining coming from landfill gas.

Of the total energy, 60 percent comes from material feedstock energy, with the remaining from fuel or process energy. Natural gas and petroleum used as raw material inputs for the production of PET are included in the PTA and EG system amounts in Table 2. The energy from these raw materials are called material feedstock energy. Figure 3 provides the breakdown of the amount of total energy required for material feedstock energy versus the process and fuel energy amounts needed to produce PET resin. As is the case for many of the plastic resins, more than half of the total energy is associated with material feedstock.

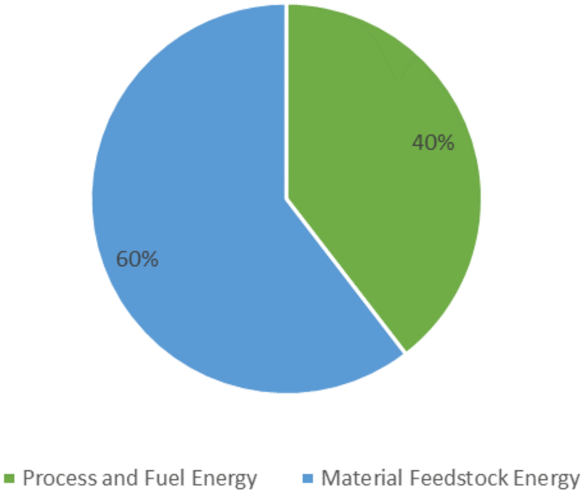

Figure 3. Energy type for PET Resin

Energy Demand by Fuel Type

Table 3 and Figure 4 provide the total energy demand by fuel type for the PET resin. Natural gas and petroleum fuels make up over 90 percent of the total energy used. As shown in Figure 3, this is partially due to the material feedstock energy (over half of the energy use) used to create the plastic. These material feedstock fuels are part of the energy shown for raw materials. The resin production energy shown in Table 3 and figure 4 represents the energy required for transportation of raw materials to resin manufacturers, the energy required to produce the resin itself, and the production of the fuels needed to manufacture the resin.

Petroleum-based fuels (e.g. diesel fuel) are the dominant energy source for transportation. Non-fossil sources, such as hydropower, nuclear and other (geothermal, wind, etc.) shown in Table 3 are used to generate purchased electricity along with the fossil fuels. Other renewable also includes a small amount of landfill gas used for process energy in ethylene production.

When reviewing the fuels used for the PTA system, over two-thirds of the energy comes from petroleum. Almost 65 percent of the PTA material inputs comes from paraxylene, which is produced from mixed xylenes created at a refinery. Material feedstock is included in this energy amount.

Almost 90 percent of the total energy from the EG system comes from natural gas. Ethylene makes up more than 50 percent of the material inputs to ethylene oxide, used to produce EG. Ninety percent of the ethylene production comes from natural gas products. Again, this amount includes material feedstock energy.

Table 3. Energy Demand by Fuel Type for PET Resin

	Basis: 1,000 pounds						
	Total Energy	**Natural Gas**	**Petroleum**	**Coal**	**Nuclear**	**Hydropower**	**Other Renewable**
	MM Btu	***MM Btu***	***MM Btu***	***MM Btu***	***MM Btu***	***MM Btu***	***MM Btu***
Cradle-to-PTA	16.7	3.90	11.4	0.76	0.51	0.054	0.075
Cradle-to-EG	7.25	6.50	0.48	0.15	0.10	0.010	0.015
PET Production	2.41	1.46	0.23	0.41	0.24	0.029	0.030
Total	**26.4**	**11.9**	**12.1**	**1.32**	**0.85**	**0.094**	**0.12**
	Basis: 1,000 kilograms						
	Total Energy	**Natural Gas**	**Petroleum**	**Coal**	**Nuclear**	**Hydropower**	**Other Renewable**
	GJ	***GJ***	***GJ***	***GJ***	***GJ***	***GJ***	***GJ***
Cradle-to-PTA	38.9	9.07	26.5	1.78	1.19	0.13	0.17
Cradle-to-EG	16.9	15.1	1.12	0.34	0.23	0.024	0.034
PET Production	5.60	3.41	0.55	0.95	0.56	0.068	0.069
Total	**61.4**	**27.6**	**28.2**	**3.07**	**1.99**	**0.22**	**0.28**
	Percentage of Total						
	Total Energy	**Natural Gas**	**Petroleum**	**Coal**	**Nuclear**	**Hydropower**	**Other Renewable**
	%	***%***	***%***	***%***	***%***	***%***	***%***
Cradle-to-PTA	63.4%	14.8%	43.3%	2.90%	1.95%	0.21%	0.28%
Cradle-to-EG	27.5%	24.6%	1.82%	0.56%	0.37%	0.04%	0.06%
PET Production	9.13%	5.55%	0.89%	1.55%	0.92%	0.11%	0.11%
Total	**100%**	**45.0%**	**46.0%**	**5.00%**	**3.24%**	**0.36%**	**0.45%**

Of the PET resin process, over 60 percent of the energy used (3.41 GJ/5.6 GJ) is from natural gas. Over two-thirds of the natural gas is combusted at the plant. Most of the remainder is combusted for the production of electricity. Petroleum comprises approximately 10 percent (0.55 GJ/5.6 GJ) of the fuel used for PET production; most of this is combusted during transport. The coal use shown is combusted for electricity use. The 2016 U.S. electricity grid is used for this study. In this grid, a little more than 30 percent of the electricity production in the US uses coal as a fuel source, while natural gas makes up approximately 34 percent of the electricity grid. The hydropower, nuclear, and other energy are all used to create electricity.

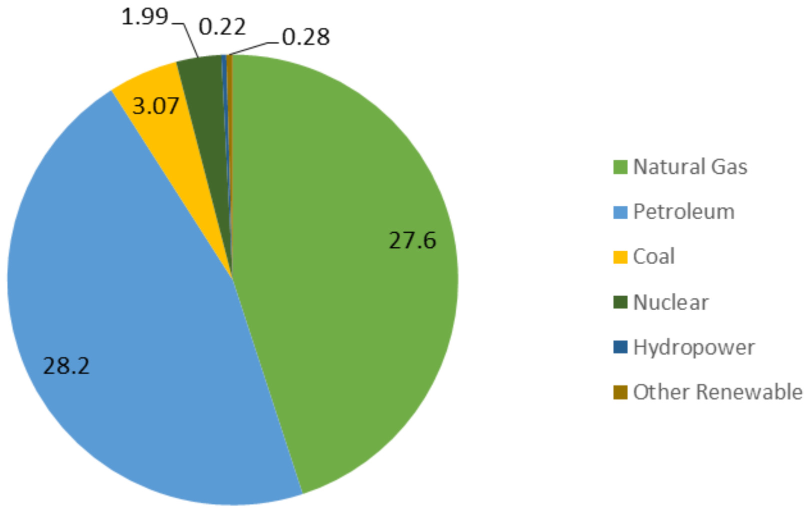

Figure 4. Energy Separated by Fuel Type for PET Resin (GJ/1,000 kg PET resin)

SOLID WASTE

Solid waste results include the following types of wastes:

- **Process wastes** that are generated by the various processes from raw material acquisition through production of PET resin (e.g., sludges and residues from chemical reactions and material processing steps)
- **Fuel-related wastes** from the production and combustion of fuels used for process energy and transportation energy (e.g., refinery wastes, coal combustion ash)

No postconsumer wastes of the resin are included in this analysis due to the use of a cradle-to-resin boundary.

The process solid waste, those wastes produced directly from the cradle-to-resin processes, includes wastes that are incinerated both for disposal and for waste-to-energy, as well as landfilled. These categories have been provided separately where possible. Solid wastes from fuel combustion (e.g. ash) are assumed to be landfilled.

Results for solid waste by weight are shown in Table 4 and Figure 5. The solid wastes have been separated in to hazardous and non-hazardous waste categories, as well as by the PTA system, EG system, and PET resin production. Approximately 18 percent of the total solid waste is created during the PET resin production, either from fuel or the PET resin process itself. Over 50 percent of the total solid waste is coming from the extraction and combustion of coal used to create electricity. Another 38 percent of the solid waste comes from the extraction of natural gas and petroleum. PET resin and each of the main intermediate chemicals (PTA, EG/EO, and Ethylene) each produce less than 3 percent of the total solid waste specifically from the manufacturing process (not including fuels).

Table 4. Solid Wastes for PET Resin

	Basis: 1,000 pounds								
		Hazardous Wastes				Non-Hazardous Wastes			
	Total Solid Waste	Waste-to-Energy	Incineration	Landfill	Hazardous Waste Total	Waste-to-Energy	Incineration	Landfill	Non-Hazardous Waste Total
	lb	*lb*	*lb*	*lb*	*lb*	*lb*	*lb*	*lb*	*lb*
Cradle-to-PTA	61.6	0	8.3E-04	0	8.3E-04	0	0.086	61.5	61.6
Cradle-to-EG	16.3	8.3E-04	0.29	6.3E-04	0.29	1.2E-04	1.45	14.6	16.0
PET Production	17.1	0	0.0048	0	0.0048	0.68	0.0034	16.5	17.1
Total	**95.0**	**8.3E-04**	**0.29**	**6.3E-04**	**0.29**	**0.68**	**1.54**	**92.5**	**94.7**
	Basis: 1,000 kilograms								
		Hazardous Wastes				Non-Hazardous Wastes			
	Total Solid Waste	Waste-to-Energy	Incineration	Landfill	Hazardous Waste Total	Waste-to-Energy	Incineration	Landfill	Non-Hazardous Waste Total
	kg	*kg*	*kg*	*kg*	*kg*	*kg*	*kg*	*kg*	*kg*
Cradle-to-PTA	61.6	0	8.3E-04	0	8.3E-04	0	0.086	61.5	61.6
Cradle-to-EG	16.3	8.3E-04	0.29	6.3E-04	0.29	1.2E-04	1.45	14.6	16.0
PET Production	17.1	0	0.0048	0	0.0048	0.68	0.0034	16.5	17.1
Total	**95.0**	**8.3E-04**	**0.29**	**6.3E-04**	**0.29**	**0.68**	**1.54**	**92.5**	**94.7**
	Percentage of Total								
		Hazardous Wastes				Non-Hazardous Wastes			
	Total Solid Waste	Waste-to-Energy	Incineration	Landfill	Hazardous Waste Total	Waste-to-Energy	Incineration	Landfill	Non-Hazardous Waste Total
	%	*%*	*%*	*%*	*%*	*%*	*%*	*%*	*%*
Cradle-to-PTA	64.8%	0%	0.001%	0%	0.001%	0%	0.1%	65%	65%
Cradle-to-EG	17.2%	0.001%	0.30%	0.001%	0.30%	0.0%	1.5%	15%	17%
PET Production	18.0%	0%	0.005%	0%	0.005%	0.7%	0.004%	17%	18%
Total	**100%**	**0.001%**	**0.31%**	**0.001%**	**0.31%**	**0.7%**	**1.6%**	**97.4%**	**99.7%**

Solid wastes are shown separated by hazardous and non-hazardous wastes in Table 4. This separation was done only where primary data was collected, or if a secondary data source was clear that the solid waste was of a hazardous nature. Much of the process solid wastes from oil and natural gas were classified as non-hazardous due to exclusions found in RCRA hazardous wastes regulations or other EPA hazardous wastes regulations. Only 0.3 percent of the total solid wastes were process hazardous wastes.

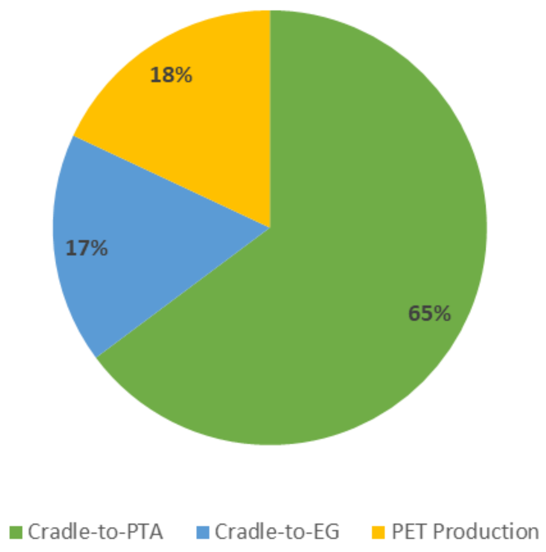

Figure 5. Solid Wastes by PTA System, EG System and PET Resin

Since the non-hazardous solid wastes make up 99.7 percent of the total solid waste, the same conclusions can be made as were made for total solid wastes previously. The hazardous wastes mainly come from the ethylene production, which makes up 87 percent of the total hazardous solid waste. Alumina production used within a catalyst for the PET production accounts for over 10 percent of the hazardous solid waste. The PET resin manufacture accounts for a little more than 1 percent of the total, while the remaining intermediate chemicals all create between 1 and 2 percent of the total hazardous solid waste.

Table 4 also provides a breakout of the total solid wastes by the disposal fate. Since much of the solid wastes come from the fuel production and combustion, over 97 percent of the total solid wastes and total non-hazardous solid waste is landfilled. Less than 1 percent of the total solid waste is used to create energy, while the remaining solid waste is incinerated with no energy capture. In the case of the hazardous solid waste, over 99 percent is incinerated with no energy capture. Minute amounts of the total hazardous solid waste are sent to waste-to-energy or landfilled.

WATER CONSUMPTION

Consumptive use of water in this study includes freshwater that is withdrawn from a water source or watershed and not returned to that source. Consumptive water use includes water consumed in chemical reactions, water that is incorporated into a product or waste stream, water that becomes evaporative loss, and water that is discharged to a different watershed or water body than the one from which it was withdrawn. Water consumption results shown for each life cycle stage include process water consumption as well as water consumption associated with production of the electricity and fuels used in that stage. Electricity-related water consumption includes evaporative losses associated with thermal generation of electricity from fossil and nuclear fuels, as well as evaporative losses due to establishment of dams for hydropower.

Water consumption results are shown in Table 5 and Figure 6. As seen in the table, 56 percent of the water consumed is from the PTA system, with 14 percent of the total directly consumed at the PTA plant. A little less than half of the water consumed in the PTA system is for the creation of electricity. In total, more than 40 percent of water consumed for the PET system does come from electricity, while another 20 percent comes from the extraction/processing of natural gas and refining of crude oil. PET resin production uses 23 percent of the total water consumed with 9 percent associated with the production of the resin at the plant and 13 percent associated with generation of electricity used in the resin production or producing the fuels used at the plant.

Table 5. Water Consumption for PET Resin

	Total Water Consumption		
	Basis: 1,000 Pounds	**Basis: 1,000 kilograms**	**Percentage of Total**
	Gallons	***Liters***	***%***
Cradle-to-PTA	524	4,376	56%
Cradle-to-EG	196	1,639	21%
PET Production	212	1,768	23%
Total	**932**	**7,783**	**100%**

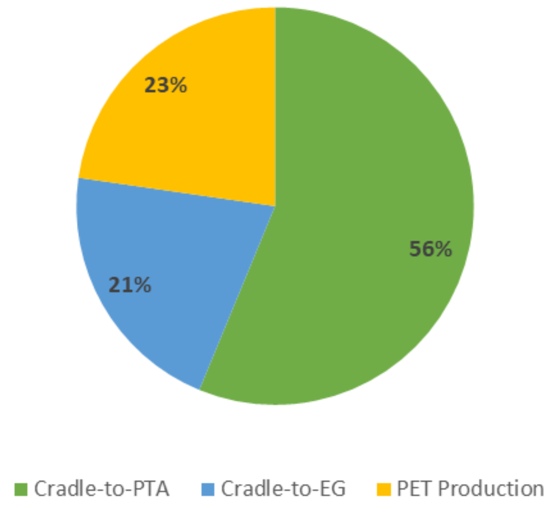

Figure 6. Water Consumption for PET Resin

GLOBAL WARMING POTENTIAL

The primary atmospheric emissions reported in this analysis that contribute over 99 percent of the total global warming potential for each system are fossil fuel-derived carbon dioxide and methane. Other contributors include nitrous oxide and some CFCs, but these contribute less than 1 percent of the total shown. Any non-fossil carbon dioxide emissions, such as those from the burning of wood-derived fuel, is a return of carbon dioxide to the atmosphere in the same form as it was originally removed from the atmosphere during the biomass growth cycle; therefore, any carbon dioxide emissions from combustion or decomposition of biomass-derived products are not considered a net contributor to global warming.

The 100-year global warming potential (GWP) factors for each of these substances as reported in the Intergovernmental Panel on Climate Change (IPCC) 2013[8] are: fossil carbon dioxide 1, fossil methane 28, and nitrous oxide 265. The GWP factor for a substance represents the relative global warming contribution of a pound of that substance compared to a pound of carbon dioxide. The weights of each greenhouse gas are multiplied by its GWP factor to arrive at the total GWP results. Although normally GWP results are closely related to the energy results, the feedstock energy is not associated with GWP due to the sequestration of the feedstock material within the plastic. It is the potential energy associated with the feedstock material, which is not combusted to create greenhouse gases.

Table 6 and Figure 7 show life cycle GWP results for the PET resin. About half of the greenhouse gas emissions and GWP for each system are fuel-related emissions rather than process emissions. Of the processes, the production of ethylene, ethylene glycol/ethylene oxide, and TPA/PTA each account for 5 to 6 percent of the total GWP results, while PX and mixed xylenes each account for more than 3 percent. The extraction and refining of petroleum comprise almost 15 percent of the total GWP.

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[8] IPCC, 2013: *Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change* [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 2013.

Table 6. Global Warming Potential for PET Resin

	Global Warming Potential		
	Basis: 1,000 Pounds	Basis: 1,000 kilograms	Percentage of Total
	lb CO2 eq	*kg CO2 eq*	*%*
Cradle-to-PTA	1,346	1,346	60%
Cradle-to-EG	534	534	24%
PET Production	354	354	16%
Total	**2,233**	**2,233**	**100%**

The PET resin production comprises 16 percent of the total GWP as seen in Table 6 and Figure 7, 96 percent of which comes from the fuel production and combustion for the process and transport, with the remaining from the mining and processing of the metals used for catalysts. Roughly half of the GWP for the PTA system is from fuel combustion, with the other half from processes (e.g. 9 percent from TPA/PTA and 23 percent from extraction/refining of petroleum). The EG system GWP includes nearly 40 percent from fuels, with the remainder from processes (e.g. 28 percent from ethylene and 20 percent from ethylene oxide/ethylene glycol).

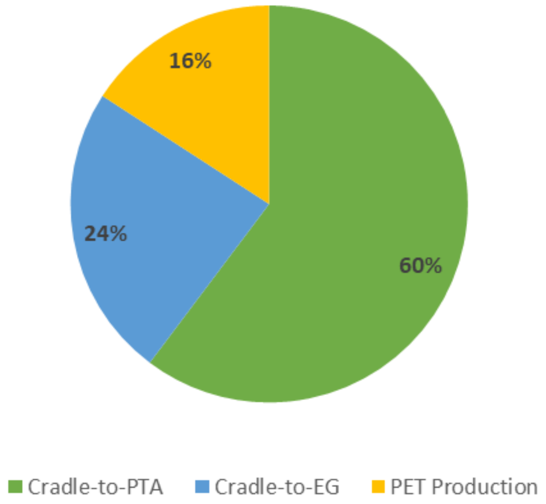

Figure 7. Global Warming Potential for PET Resin

ACIDIFICATION POTENTIAL

Acidification assesses the potential of emissions to contribute to the formation and deposit of acid rain on soil and water, which can cause serious harm to plant and animal life as well as damage to infrastructure. Acidification potential modeling in TRACI incorporates the results of an atmospheric chemistry and transport model, developed by the U.S. National Acid Precipitation Assessment Program (NAPAP), to estimate total North American terrestrial deposition due to atmospheric emissions of NO_x and SO_2, as a function of the emissions location.[9,10]

Acidification impacts are typically dominated by fossil fuel combustion emissions, particularly sulfur dioxide (SO_2) and nitrogen oxides (NO_x). Emissions from combustion of fossil fuels, especially coal, to generate grid electricity is a significant contributor to acidification impacts for all systems. Table 7 shows total acidification potential (AP) results for the PET resin. Results are shown graphically in Figure 8.

The PET resin production comprises 29 percent of the total AP, almost all of which comes from the fuel production and combustion for the process and transport. The AP from the PET process makes up less than 1 percent of the total AP, with 4 percent coming from the mining and processing of metals used for catalysts. Over 80 percent of the AP amount for the PTA system is from fuels used in the processes and transport. Of the remaining percentage, 15 percent comes from the production of oil and gas for material use. Of the AP amount (17 percent of the total AP for the PET resin system) for the EG system, half comes from the production of oil and gas for material use. More than 40 percent of the AP portion from the EG system comes from fuel production and combustion, with the remaining coming from the production of intermediate chemicals.

Table 7. Acidification Potential for PET Resin

	Acidification Potential		
	Basis: 1,000 Pounds	Basis: 1,000 kilograms	Percentage of Total
	lb SO2 eq	*kg SO2 eq*	*%*
Cradle-to-PTA	3.92	3.92	54%
Cradle-to-EG	1.21	1.21	17%
PET Production	2.10	2.10	29%
Total	**7.24**	**7.24**	**100%**

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[9] Bare JC, Norris GA, Pennington DW, McKone T. (2003). TRACI: The Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts, *Journal of Industrial Ecology,* **6**(3–4): 49–78. Available at URL: http://mitpress.mit.edu/journals/pdf/jiec_6_3_49_0.pdf.

[10] Bare JC. (2002). Developing a consistent decision-making framework by using the US EPA's TRACI, AICHE. Available at URL: http://www.epa.gov/nrmrl/std/sab/traci/aiche2002paper.pdf.

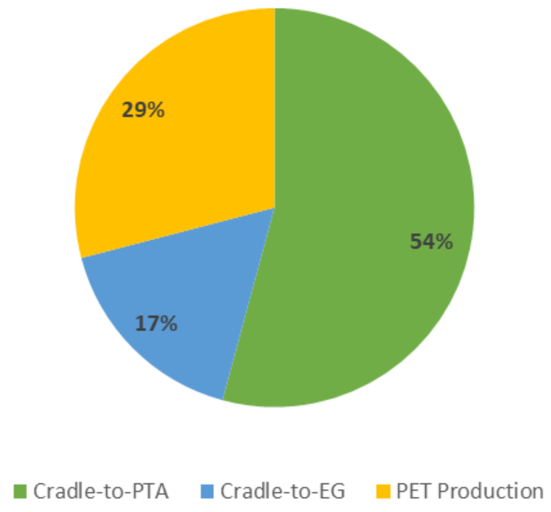

Figure 8. Acidification Potential for PET Resin

EUTROPHICATION POTENTIAL

Eutrophication occurs when excess nutrients are introduced to surface water causing the rapid growth of aquatic plants. This growth (generally referred to as an “algal bloom”) reduces the amount of dissolved oxygen in the water, thus decreasing oxygen available for other aquatic species. The TRACI characterization factors for eutrophication are the product of a nutrient factor and a transport factor.[11] The nutrient factor is based on the amount of plant growth caused by each pollutant, while the transport factor accounts for the probability that the pollutant will reach a body of water. Atmospheric emissions of nitrogen oxides (NO_x) as well as waterborne emissions of nitrogen, phosphorus, ammonia, biochemical oxygen demand (BOD), and chemical oxygen demand (COD) are the main contributors to eutrophication impacts.

Eutrophication potential (EP) results for PET resin are shown in Table 8 and illustrated in Figure 9. The PET resin production accounts for 51 percent of the EP impact. Almost 27 percent of the total comes from the antimony mining and processing used to create one of the PET catalysts. Of the remaining 24 percent created from in the PET resin production, 2/3 of this comes from fuel production and combustion for process and transport account with the remaining amount from the PET resin process emissions (8 percent of the total EP).

The natural gas and crude oil extraction and processing/refining create 20 percent of the total EP, while the combustion of fuels for boilers and transport make up more than 30 percent of the total EP. Of the approximately 15 percent of the EP created by emissions at

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[11] Bare JC, Norris GA, Pennington DW, McKone T. (2003). TRACI: The Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts, *Journal of Industrial Ecology,* **6**(3–4): 49–78. Available at URL: http://mitpress.mit.edu/journals/pdf/jiec_6_3_49_0.pdf.

the unit processes, PET resin production releases more than half. This is due to the waterborne release of nitrogen and phosphate, as well as BOD and COD amounts, as shown in the PET resin average shown in the Appendix of this report. The nitrogen and phosphates emissions were provided by less than three plants and so an order of magnitude was used as a surrogate amount. It is anticipated that the EP may increase or decrease by a small percentage (1-2 percent) if data were available from all plants.

Table 8. Eutrophication Potential for PET Resin

	Eutrophication Potential		
	Basis: 1,000 Pounds	**Basis: 1,000 kilograms**	**Percentage of Total**
	lb N eq	***kg N eq***	***%***
Cradle-to-PTA	0.16	0.16	35%
Cradle-to-EG	0.061	0.061	14%
PET Production	0.23	0.23	51%
Total	**0.45**	**0.45**	100%

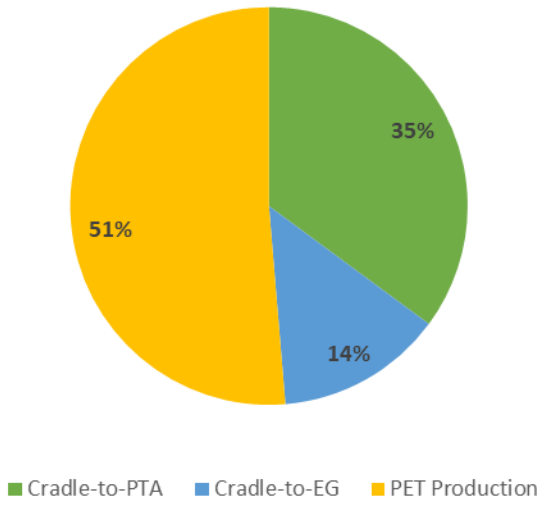

Figure 9. Eutrophication Potential for PET Resin

OZONE DEPLETION POTENTIAL

Stratospheric ozone depletion (ODP) is the reduction of the protective ozone within the stratosphere caused by emissions of ozone-depleting substance (e.g. CFCs and halons). The ozone depletion impact category characterizes the potential to destroy ozone based on a chemical's reactivity and lifetime. Damage related to ozone depletion can include skin cancer, cataracts, material damage, immune system suppression, crop damage, and other plant and animal effects.

Table 9 shows total ODP results for PET resin, which are also shown graphically in Figure 10. Ozone depletion results for the PET resin are dominated by the production of TPA/PTA system, contributing 99.6 percent of the total ozone depletion impacts. This is specifically due to the release of methylbromide at the TPA/PTA (98 percent of that 99.6 percent), PX, and oil refining plants. At the PTA and PX plants, the methylbromide emission amounts were provided by less than three plants and so an order of magnitude was used as a surrogate amount in the average. The ozone depletion may increase or decrease if all plants provided data; however, the percentage change in ODP is unknown. The remaining ozone depletion impacts are primarily associated with the metals used for catalysts in PET production and the extraction and combustion of fuels.

Table 9. Ozone Depletion Potential for PET Resin

	Ozone Depletion Potential		
	Basis: 1,000 Pounds	**Basis: 1,000 kilograms**	**Percentage of Total**
	lb CFC-11 eq	***kg CFC-11 eq***	***%***
Cradle-to-PTA	4.5E-04	4.5E-04	99.6%
Cradle-to-EG	2.5E-07	2.5E-07	0.06%
PET Production	1.7E-06	1.7E-06	0.38%
Total	**4.5E-04**	**4.5E-04**	**100%**

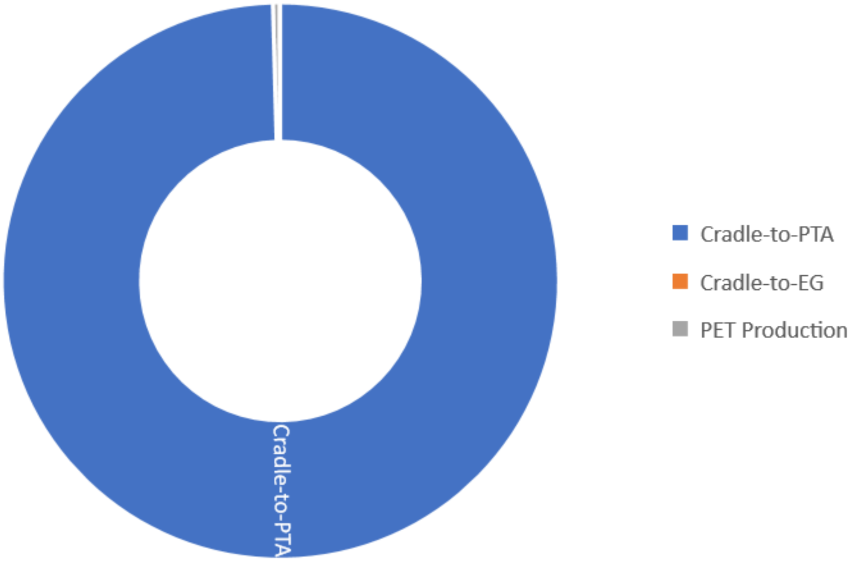

Figure 10. Ozone Depletion Potential for PET Resin

PHOTOCHEMICAL SMOG FORMATION

The photochemical smog formation (POCP) impact category characterizes the potential of airborne emissions to cause photochemical smog. The creation of photochemical smog occurs when sunlight reacts with NO_x and volatile organic compounds (VOCs), resulting in tropospheric (ground-level) ozone and particulate matter. Endpoints of such smog creation can include increased human mortality, asthma, and deleterious effects on plant growth. Smog formation impact are generally dominated by emissions associated with fuel combustion, so that impacts are higher for life cycle stages and components that have higher process fuel and transportation fuel requirements. In this case, NO_x makes up more than 92 percent of the smog formation emissions, with VOCs consisting of another 6 percent.

Over 50 percent of the PCOP comes from fuel use in processes and transport. Furthermore, natural gas and crude oil extraction create the emissions leading to 38 percent of the PCOP. The remainder (almost 7 percent) of the PCOP is created from unit processes with one percent coming from the production of ethylene.

Smog formation potential results for the PET resin are displayed in Table 10 and illustrated in Figure 11. More than half of the emissions that have the potential to create smog come from the PTA system. In the PTA system, the PCOP is created from approximately the same split as the total PCOP (estimated 60 percent from fuels and 33 percent from extraction of oil and gas). In the EG system, over 70 percent of the PCOP results come from the extraction of oil and gas, with a little less than 20 percent from fuels.

For the PET resin production, emissions from combustion of transport fuels release more than half of those smog formation emissions. Only one percent of the PCOP coming from the PET production is from the process itself, as well as one percent of the PCOP comes from the mining and processing of metals for use in catalysts for PET resin production. The remaining 98 percent comes from fuel production and use for the process and the transport. Within this amount, electricity production at the PET production facility releases over 20 percent of the production of the emissions creating the smog formation potential.

Table 10. Photochemical Smog Formation Potential for PET Resin

	Photochemical Smog Potential		
	Basis: 1,000 Pounds	**Basis: 1,000 kilograms**	**Percentage of Total**
	lb O3 eq	***kg O3 eq***	***%***
Cradle-to-PTA	81.2	81.2	54%
Cradle-to-EG	30.3	30.3	20%
PET Production	38.4	38.4	26%
Total	**150**	**150**	**100%**

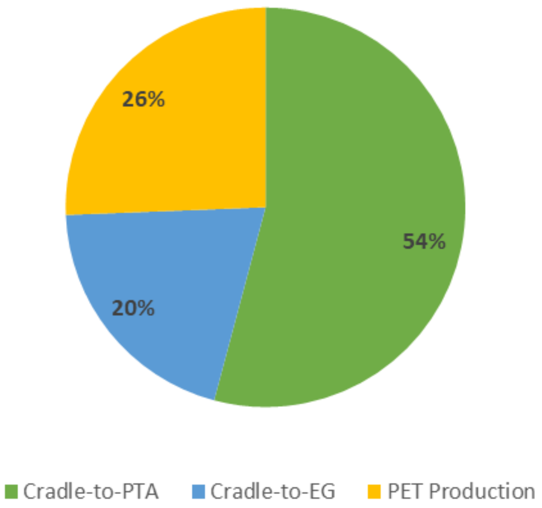

Figure 11. Smog Formation Potential for PET Resin

COMPARISON OF 2018 AND 2011 LCI AND LCIA RESULTS

This section provides a comparison of life cycle inventory and impact assessment category results that were included in the original virgin PET system[12] with the current update. These categories include total energy, non-renewable energy, renewable energy, total solid waste, and global warming potential. No comparisons are available for water consumption, solid waste broken out as hazardous and non-hazardous categories, acidification potential, eutrophication potential, photochemical smog formation, or ozone depletion potential. These categories were not included in the original study.

Table 11 shows the comparable LCI and LCIA categories for the 2011 and 2018 in both English and SI units and includes the percent change from the original results for each category. The percent change equals the difference of the two amounts divided by the 2011 original result. From the results, an overall decrease is seen across the comparable LCI and LCIA categories included for both the original 2011 and the new 2018 analysis. Comparisons of these results have been analyzed in this section focusing on the main differences causing the decrease in each category. Broadly, results differences fall into three types:

1. Different manufacturing plants were used in replaced primary data
2. New primary data
3. Exclusion of DMT-based PET

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[12] American Chemistry Council, Plastics Division, Cradle-to-Gate Life Cycle Inventory of Nine Plastic Resins and Four Polyurethane Precursors. Prepared by Franklin Associates, A Division of ERG. August, 2011.

Table 11. Comparison of 2011 and 2018 LCI and LCIA Results for Virgin PET Resin

	1000 pounds of Virgin Polyethylene Terephthalate Resin				
	LCI Results				*LCIA Results*
	Total Energy	Non-Renewable Energy	Renewable Energy	Total Solid Waste	Global Warming
	MM Btu	*MM Btu*	*MM Btu*	*lb*	*lb CO_2 eq*
PET 2018	26.4	26.2	0.21	95.1	2,233
PET 2011	30.3	30.0	0.28	141	2,733

	1000 kilograms of Virgin Polyethylene Terephthalate Resin				
	LCI Results				*LCIA Results*
	Total Energy	Non-Renewable Energy	Renewable Energy	Total Solid Waste	Global Warming
	GJ	*GJ*	*GJ*	*kg*	*kg CO_2 eq*
PET 2018	61.4	60.9	0.50	95.1	2,233
PET 2011	70.4	69.8	0.65	141	2,733
Percent Change	-13%	-13%	-24%	-33%	-18%

1. **Different manufacturing plants were used for the processes where primary data was collected in both studies.** Each plant producing the same resin or chemical varies by the amounts of materials used, fuel types and amounts used, amounts of emissions released, etc. All these changes lead to differences affecting the results. Data were collected for PET resin, TPA/PTA, and ethylene in 2004-2006. For ethylene and PTA, a couple of the same plants were included; however, most of the plants in the averages were not included in the original data collection. Also, more plants participated in this update, allowing two separate averages for PET and TPA/PTA, whereas these plants were combined in the original study.

2. **New primary data was used in place of either older primary data or secondary data.** In the case of paraxylene, ethylene oxide and ethylene glycol, no inventory data was collected in the original study. Paraxylene data came from a secondary source, while EO/EG data were collected in the early 1990s. Updating these data allowed for changes in technology, efficiency increases, and changes in fuel use. These updates caused the largest decreases in the PET resin results.

3. **2011 PET results included a percentage of DMT-based PET.** PET results in the 2011 analysis were a split of 85 percent PTA-based PET and 15 percent DMT-based PET. These intermediate chemicals are created by very different processes. Also, data were collected for PTA, while the DMT data were from primary sources from the early 1990s.

ENERGY COMPARISON

Overall, the total and non-renewable energy has decreased 9.0 GJ on a 1,000 kg basis (3.9 MMBtu/1,000 lb). This is a 13 percent decrease in total and non-renewable energy as compared to the original results, which is larger than could normally be explained by efficiency improvements or small decreases in required input materials. Most of this decrease is due to the three points discussed earlier in this section. Figure 12 provides a graphical perspective of the unit processes associated with the total energy decrease from the original energy amounts.

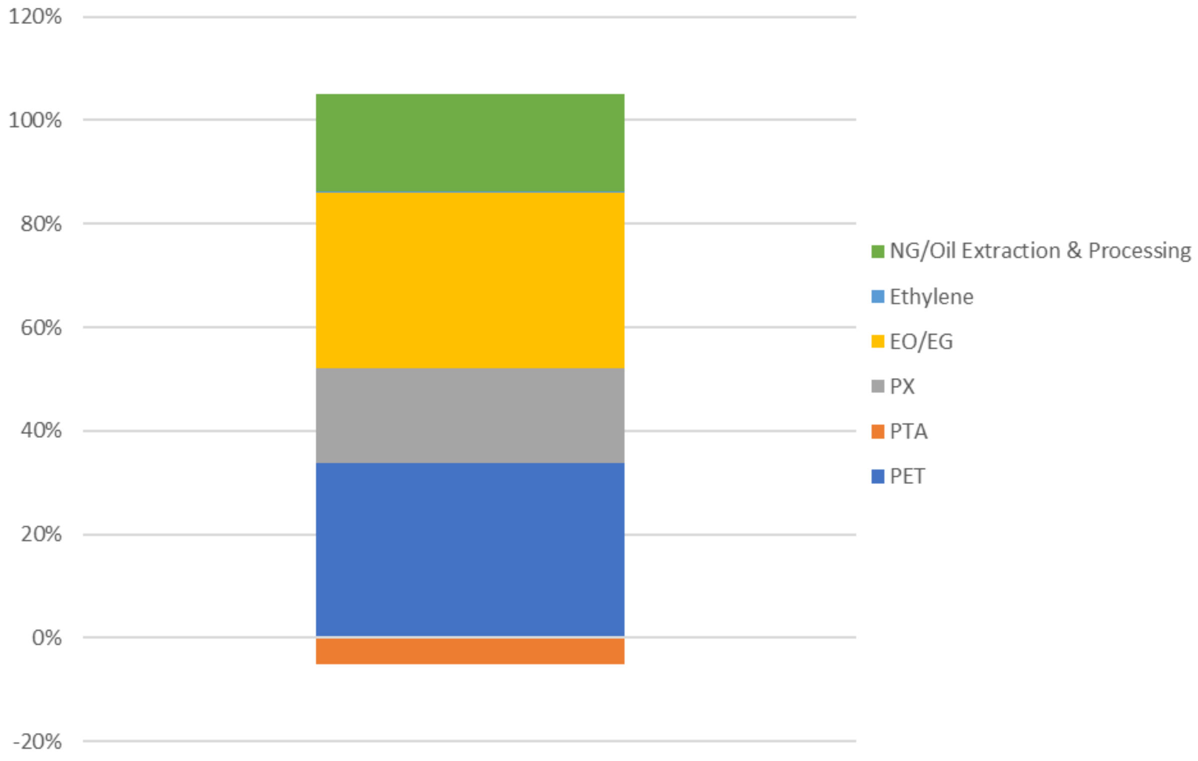

Figure 12. Decrease in Total Energy by Unit Process (percent of total)

Specifically, the largest decrease in total and non-renewable energy is due to the collected PET resin unit process, which showed improvement in energy use. The PET resin unit process decreased by 3.2 GJ/1000 kg PET. Possibly this decrease is due to efficiency or technological improvements, or this could be due to differences in the plants that collected data, as the original plants did not participate in this analysis. The EO/EG process dataset also showed improvement in energy use. This improvement in EO/EG data decreased the energy for the PET system by approximately 2.8 GJ/1000 kg PET. The use of primary data for paraxylene and updated secondary data for the extraction and processing of natural gas and petroleum also decreased the energy for PET resin system by approximately 1.8 GJ/1000 kg PET resin each. The PTA primary data was more robust than the original, which only included data from 2 plants and was combined with 2 PET plants in the 2011 results. The energy results for PTA increased by approximately 0.5 GJ/1000 kg PET, which could be due to differences in plant fuels and efficiencies. The results from the ethylene data were very similar to the previous analysis, showing a small decrease in energy compared to the original results.

The difference in renewable energy is a 24 percent decrease from the original amount. Although this seems quite large, the renewable energy makes up less than one percent of the total energy. The unit processes that changed the greatest amount from the original PET renewable energy are the EO/EG and oil extraction and refining. The decrease in these comes mostly from a drop in the electricity amount used for the processes.

SOLID WASTE COMPARISON

When compared to the 2011 PET resin total solid waste amount, the current PET resin study creates over 46 kg/1000 kg PET less solid waste, which is a 33 percent drop. Again, this drop is likely due to the 3 points previously discussed. Figure 13 provides a visual of the amounts for all unit processes that make up the decrease in total solid waste. The largest part of the decrease comes from the PET process. This could be due to improvements in the process over the past 10 years but could also be due to the collection of data from completely different plants than the previous study. The same conclusion can be made about the decrease in solid waste shown in the PTA and EO/EG processes. The PX solid waste decrease is likely due to improvements in available primary data sources.

GLOBAL WARMING POTENTIAL COMPARISON

The global warming potential decreased by 500 kg CO_2 equivalents/1000 kg PET resin, or 18 percent compared to the 2011 PET resin GWP result. Figure 14 displays a column chart with the unit processes that makeup the decrease in GWP when comparing the 2011 and 2018 GWP results. For the most part, this decrease follows the decrease in total energy, since much of the greenhouse gases are created from fuel production. However, focusing on the unit processes in the PET system, the natural gas and crude oil category shows an increase (depicted as a negative percentage on Figure 14). In this case, the more recent oil extraction data shows a higher amount of greenhouse gas emissions released during the process than those in the previous oil extraction dataset. The GWP from the PTA process also increases, but this increase is expected due to the increase in energy use.

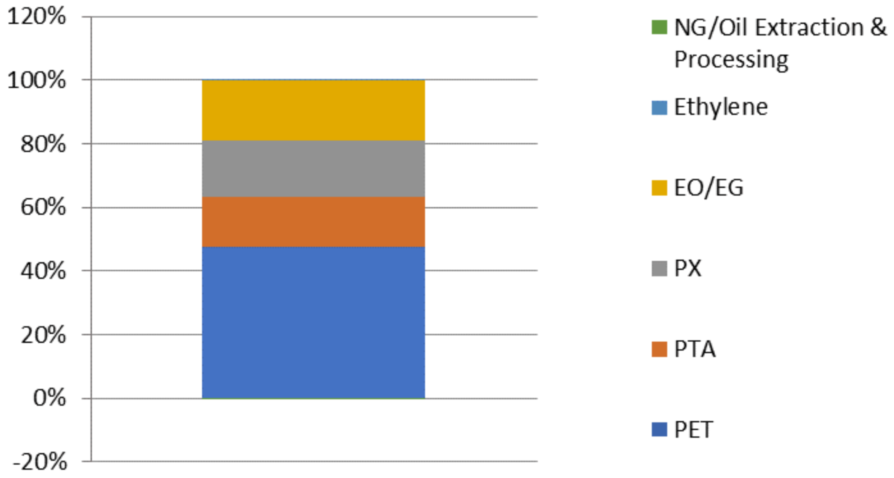

Figure 13. Decrease in Solid Waste Weight by Unit Process (percent of total)

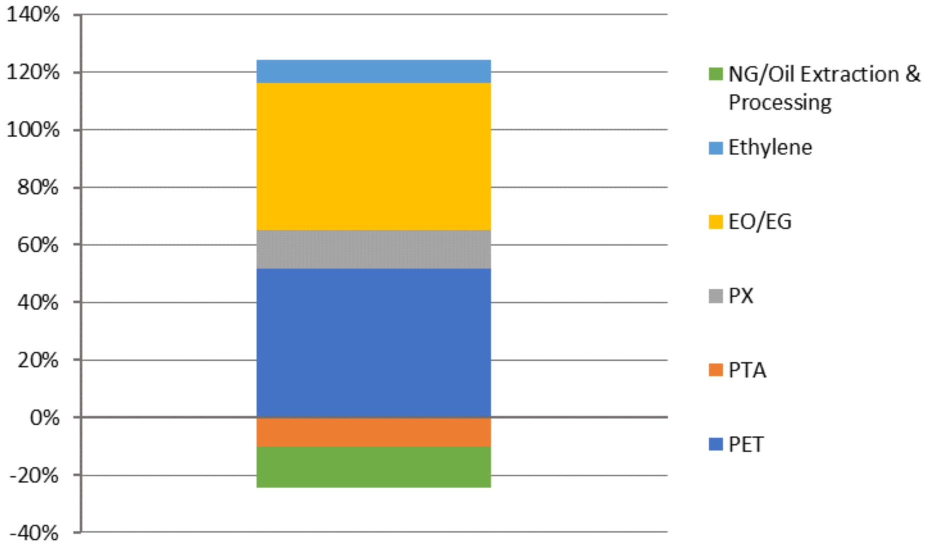

Figure 14. Decrease in Global Warming Potential by Unit Process (percent of total)

APPENDIX: POLYETHYLENE TEREPHTHALATE MANUFACTURE

This appendix discusses the manufacture of polyethylene terephthalate (PET) resin. Examples of PET resin end-uses include consumer food product packaging, beverage containers, and personal care products. Approximately 4.7 million tons of polyethylene terephthalate capacity was available in 2015 in North America (Plastics Insight, 2016). The material flow for PET resin is shown in Figure 2 in the Goal and Scope section. Individual unit process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. The following processes are included in this appendix:

- Crude oil production
- Petroleum refining
- Natural gas production
- Natural gas processing
- Olefins production (Ethylene)
- Oxygen production
- Ethylene oxide/Ethylene glycol production
- Methanol production
- Carbon monoxide production
- Mixed xylenes production
- Paraxylene production
- Crude terephthalic acid (TPA)/Purified terephthalic acid (PTA) production
- Polyethylene terephthalate melt phase & solid phase resin production

LCI data for many of the processes listed above were collected for this update to the U.S. LCI plastics database by NAPCOR member companies, as well as member companies of the American Chemistry Council (ACC). These processes include olefin production, ethylene oxide/ethylene glycol production, paraxylene production, TPA/PTA production, and PET resin production. Secondary or previously collected primary data was used for crude oil extraction and refining, natural gas production and processing, carbon monoxide, methanol and oxygen.

A flow diagram of the production of solid-state PET resin is shown in Figure 15. Processes that are provided as an aggregated data set are enclosed by a dashed line box. Aggregation was done in some cases to protect confidential data, while in other cases due to provision of integrated plant data.

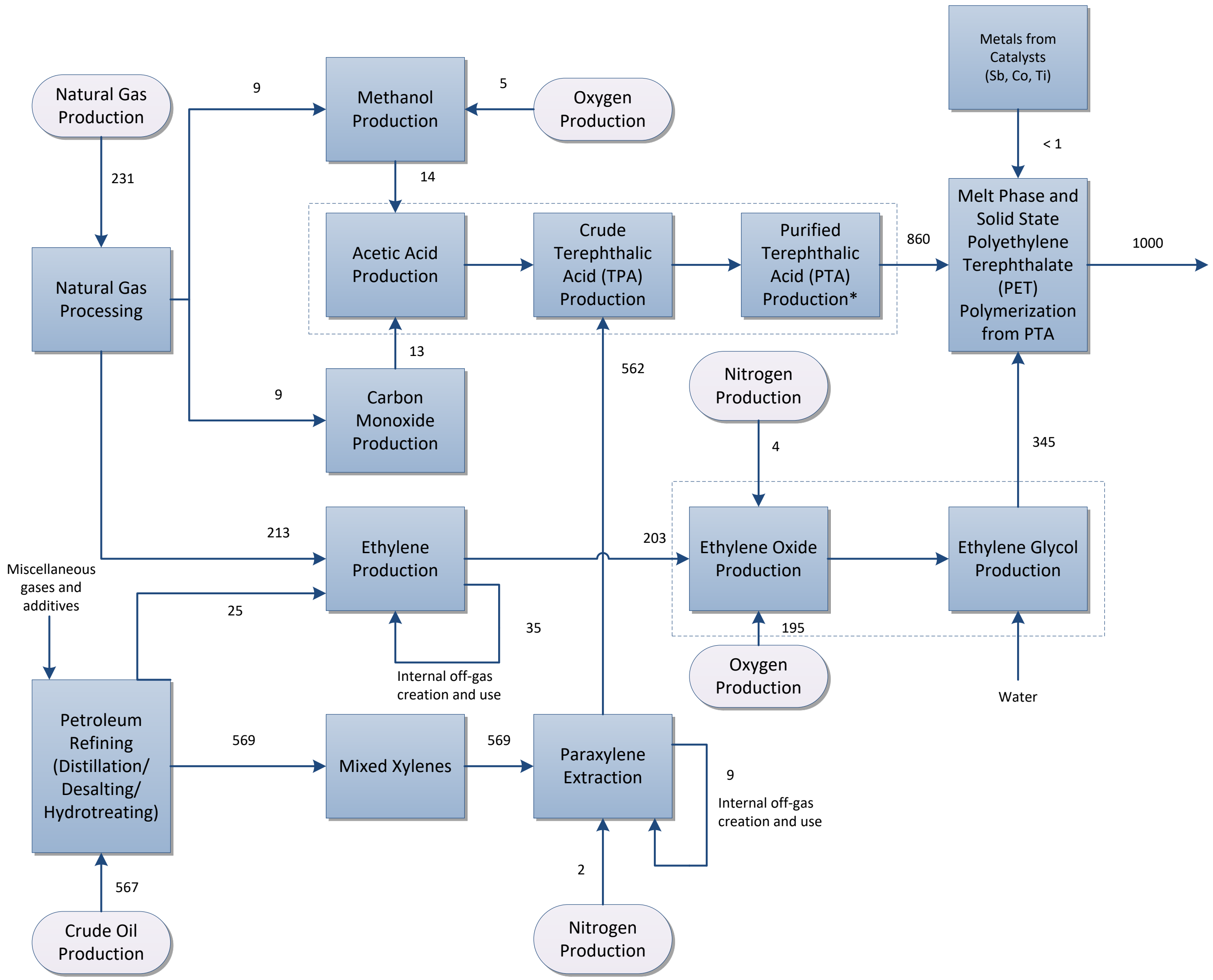

Figure 15. Flow diagram for the production of 1,000 pounds/1,000 kilograms solid-state PET resin.
Note: Metals mining and processing from the catalysts have also been included but are not shown here.

CRUDE OIL EXTRACTION

Oil is produced by drilling into porous rock structures generally located several thousand feet underground. Once an oil deposit is located, numerous holes are drilled and lined with steel casing. Some oil is brought to the surface by natural pressure in the rock structure, although most oil requires energy to drive pumps that lift oil to the surface. Once oil is on the surface, it is separated from water and stored in tanks before being transported to a refinery. In some cases, it is immediately transferred to a pipeline that transports the oil to a larger terminal.

The U.S. crude oil production is made up of domestic on-shore, domestic off-shore, imported on-shore and imported off-shore sources. Based on the 2014 national average petroleum supply chain, LCI data is calculated using pollutant emission records from the National Emissions Inventory (NEI), domestic petroleum production data, and imported oil data. Table 12 provides the percentages for each type of crude oil extraction source as used for this unit process data set.

Table 12. Percentage Contribution by Source to Crude Oil Extraction Mix

Domestic Onshore	Domestic Offshore	Foreign Onshore	Foreign Offshore
42.36%	8.75%	38.55%	10.33%

Sources: US EPA 2017, US EIA 2017a, Sheridan 2006, NOAA 2017, BOEM 2017, US EIA 2017b, US EIA 2017c

The data for this unit process provides a summary of relevant input and output flows associated with extraction of domestic and imported crude oil and condensate. The data set takes into account domestic onshore extraction, domestic offshore extraction, foreign onshore extraction, and foreign offshore extraction based on the percentages provided in Table 12. The energy inputs of this process are taken from GREET model 2017 (ANL, 2017). These inputs include energy from natural gas, petroleum and other fossil fuels in addition to electricity use. The energy inputs are assumed to be the same for the domestic and imported on-shore and off-shore extraction processes. Table 13 shows the energy requirements for the extraction of 1,000 pounds and 1,000 kilograms of crude oil as per the GREET 2017 model.

The emission data for the process is adapted from inventory data compiled by the National Energy Technology Lab. The following briefly summarizes that data collection effort as documented in Young et. al. 2019. The inventory for crude oil extraction accounts for emissions to air as reported in the NEI for U.S. extraction sites, greenhouse gas emissions from Cooney et. al. 2017, and emissions to water from EPA's Discharge Monitoring Reports. Non-GHG emissions inventories for foreign oil extraction are unavailable so were assumed to scale linearly according to changes in carbon dioxide emission from domestic extraction. Emissions data from each U.S. county were allocated between oil extraction and natural gas based on North American Industry Classification System (NAICS) and source classification codes included in the NEI. For cases in which not enough detail was provided from emissions records, emissions were allocated between oil and gas in that county based on the energy content of reported production.

Table 13. Energy Requirements for the Extraction of Crude Oil

	1,000 lb		1,000 kg	
Energy				
Process Energy				
Electricity from grid	16.4	kWh	36.3	kWh
Natural gas	0.28	ft^3	0.018	m^3
Gasoline	0.063	gal	5.3E-04	m^3
Diesel	0.44	gal	0.0037	m^3
Residual Oil	0.027	gal	2.2E-04	m^3
Distillate Oil	0.027	gal	2.2E-04	m^3

Sources: ANL, 2017

Solid wastes include drilling wastes and associated wastes as calculated from statistics in EPA 2000 and API 2000. Drilling wastes include solids from brine water and drilling mud, while associated wastes are tank bottoms, contaminated soil and scale or sludges from radioactive materials.

No information was found pertaining to fresh water consumption used in onshore or offshore extraction, and so this is not included. Water is extracted with the oil and is called produced water. This produced water is a brine and so not included as consumed water.

Table 14 through Table 17 provide the emissions for 1,000 pounds and 1,000 kilograms of crude oil extraction by source (onshore domestic, offshore domestic, onshore foreign, and offshore foreign).

Table 14. Environmental Emissions for the Extraction of Crude Oil (Onshore Domestic)

	1,000 lb	1,000 kg
Environmental Emissions		
Atmospheric Emissions		
Carbon dioxide	343 lb	343 kg
Benzene, ethyl-	0.00 lb	0.00 kg
Styrene	0.000 lb	0.000 kg
Benzene, 1,4-dichloro-	0.00 lb	0.00 kg
Ethane, 1,2-dibromo-	1.0E-05 lb	1.0E-05 kg
Butadiene	3.7E-04 lb	3.7E-04 kg
Acrolein	0.0018 lb	0.0018 kg
Ethane, 1,2-dichloro-	4.7E-07 lb	4.7E-07 kg
Ethylene glycol	2.0E-08 lb	2.0E-08 kg
4-Methyl-2-pentanone	2.5E-06 lb	2.5E-06 kg
m-Xylene	3.8E-07 lb	3.8E-07 kg
Toluene	0.015 lb	0.015 kg
Benzene, chloro-	8.5E-06 lb	8.5E-06 kg
Phenol	4.5E-06 lb	4.5E-06 kg
Ethanol, 2-methoxy-	2.3E-07 lb	2.3E-07 kg
Hexane	0.0019 lb	0.0019 kg
Ethanol, 2-ethoxy-	7.1E-12 lb	7.1E-12 kg
Diethanolamine	9.5E-08 lb	9.5E-08 kg
Anthracene	3.0E-09 lb	3.0E-09 kg
1,4-Dioxane	1.0E-07 lb	1.0E-07 kg
Ethene, tetrachloro-	2.5E-06 lb	2.5E-06 kg
Pyrene	7.2E-09 lb	7.2E-09 kg
Hydrocarbons, aromatic	3.8E-06 lb	3.8E-06 kg
Cresol	1.2E-09 lb	1.2E-09 kg
Xylene	0.0038 lb	0.0038 kg
Chromium III	7.3E-07 lb	7.3E-07 kg
t-Butyl methyl ether	8.4E-11 lb	8.4E-11 kg
Glycol ethers	2.2E-08 lb	2.2E-08 kg
Arsenic, ion	1.2E-06 lb	1.2E-06 kg
Chromium VI	3.4E-07 lb	3.4E-07 kg
Benzo(g,h,i)perylene	1.7E-06 lb	1.7E-06 kg
Benzo(e)pyrene	1.3E-09 lb	1.3E-09 kg
Indeno(1,2,3-cd)pyrene	2.0E-10 lb	2.0E-10 kg
Perylene	1.5E-11 lb	1.5E-11 kg
Benzo(b)fluoranthene	8.4E-10 lb	8.4E-10 kg
Fluoranthene	7.4E-09 lb	7.4E-09 kg
Benzo(k)fluoranthene	1.5E-10 lb	1.5E-10 kg
Acenaphthylene	2.7E-08 lb	2.7E-08 kg
Chrysene	4.7E-09 lb	4.7E-09 kg
Hydrazine	3.9E-15 lb	3.9E-15 kg
Cyanamide	1.3E-09 lb	1.3E-09 kg
Carbonyl sulfide	1.2E-04 lb	1.2E-04 kg

Table 14. Environmental Emissions for the Extraction of Crude Oil (Onshore Domestic) (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
*Atmospheric Emissions ***				
Formaldehyde	0.017	lb	0.017	kg
Benzo(a)pyrene	1.6E-09	lb	1.6E-09	kg
Dibenz(a,h)anthracene	2.1E-10	lb	2.1E-10	kg
Pentane, 2,2,4-trimethyl-	1.6E-04	lb	1.6E-04	kg
Propene, 1,3-dichloro-	6.7E-06	lb	6.7E-06	kg
Methane, tetrachloro-, CFC-10	8.7E-06	lb	8.7E-06	kg
3-Methylcholanthrene	5.9E-11	lb	5.9E-11	kg
Benzo(a)anthracene	1.7E-07	lb	1.7E-07	kg
7,12-Dimethylbenz(a)anthracene	5.2E-10	lb	5.2E-10	kg
Carbon monoxide	0.63	lb	0.63	kg
Methanol	0.0020	lb	0.0020	kg
Chloroform	7.2E-06	lb	7.2E-06	kg
Benzene	0.024	lb	0.024	kg
Ethane, 1,1,1-trichloro-, HCFC-140	1.3E-05	lb	1.3E-05	kg
Lead	3.9E-06	lb	3.9E-06	kg
Manganese	4.7E-07	lb	4.7E-07	kg
Mercury	9.4E-08	lb	9.4E-08	kg
Nickel	4.3E-06	lb	4.3E-06	kg
Beryllium	3.7E-08	lb	3.7E-08	kg
Cadmium	1.3E-07	lb	1.3E-07	kg
Cobalt	4.7E-09	lb	4.7E-09	kg
Sulfur dioxide	0.082	lb	0.082	kg
Methane, bromo-, Halon 1001	1.1E-12	lb	1.1E-12	kg
Methane, monochloro-, R-40	4.2E-11	lb	4.2E-11	kg
Ethane, chloro-	8.0E-08	lb	8.0E-08	kg
Ethene, chloro-	4.4E-06	lb	4.4E-06	kg
Acetaldehyde	0.0021	lb	0.0021	kg
Methane, dichloro-, HCC-30	2.5E-05	lb	2.5E-05	kg
Carbon disulfide	6.4E-07	lb	6.4E-07	kg
Ethylene oxide	5.3E-11	lb	5.3E-11	kg
Ethane, 1,1-dichloro-	5.9E-06	lb	5.9E-06	kg
Ethene, 1,1-dichloro-	1.2E-09	lb	1.2E-09	kg
Propylene oxide	3.2E-07	lb	3.2E-07	kg
Hydrogen chloride	5.3E-07	lb	5.3E-07	kg
Ammonia	2.7E-04	lb	2.7E-04	kg
Phosphorus	8.7E-07	lb	8.7E-07	kg
Selenium	1.7E-07	lb	1.7E-07	kg
Chlorine	1.8E-07	lb	1.8E-07	kg
Hydrogen sulfide	4.3E-04	lb	4.3E-04	kg
Propane, 1,2-dichloro-	6.8E-06	lb	6.8E-06	kg
Ethane, 1,1,2-trichloro-	8.0E-06	lb	8.0E-06	kg
Ethene, trichloro-	4.8E-08	lb	4.8E-08	kg

Table 14. Environmental Emissions for the Extraction of Crude Oil (Onshore Domestic) (continued)

	1,000 lb	1,000 kg
Environmental Emissions		
Atmospheric Emissions		
Acrylamide	3.3E-11 lb	3.3E-11 kg
Ethane, 1,1,2,2-tetrachloro-	1.4E-05 lb	1.4E-05 kg
Acenaphthene	9.1E-09 lb	9.1E-09 kg
Phenanthrene	5.2E-08 lb	5.2E-08 kg
Fluorene	2.7E-08 lb	2.7E-08 kg
Naphthalene	5.4E-05 lb	5.4E-05 kg
Naphthalene, 2-methyl-	1.7E-07 lb	1.7E-07 kg
Biphenyl	9.1E-06 lb	9.1E-06 kg
o-Xylene	7.8E-08 lb	7.8E-08 kg
Cumene	1.5E-08 lb	1.5E-08 kg
Acetophenone	8.8E-10 lb	8.8E-10 kg
Nitrogen oxides	0.45 lb	0.45 kg
Particulates, > 2.5 um, and < 10um	3.2E-04 lb	3.2E-04 kg
Particulates, < 2.5 um	0.013 lb	0.013 kg
VOC, volatile organic compounds	4.37 lb	4.37 kg
Waterborne Releases		
Dissolved solids	0.027 lb	0.027 kg
Suspended solids, unspecified	0.0067 lb	0.0067 kg
Sulfate	0.010 lb	0.010 kg
Chloride	0.0016 lb	0.0016 kg
Hydrocarbons, aromatic	1.9E-04 lb	1.9E-04 kg
Ammonia	4.8E-05 lb	4.8E-05 kg
Manganese	3.5E-05 lb	3.5E-05 kg
Oils, unspecified	3.3E-05 lb	3.3E-05 kg
Fluoride	4.3E-06 lb	4.3E-06 kg
Bromide	2.1E-07 lb	2.1E-07 kg
Copper	5.6E-08 lb	5.6E-08 kg
Chlorine	6.5E-10 lb	6.5E-10 kg
Zinc	1.9E-08 lb	1.9E-08 kg
Benzene, ethyl-	7.6E-10 lb	7.6E-10 kg
Mercury	8.3E-11 lb	8.3E-11 kg
Radium-226	3.9E-21 Cu	1.5E-13 kBq
Sulfide	7.2E-05 lb	7.2E-05 kg
Toluene	5.2E-09 lb	5.2E-09 kg
Xylene	6.4E-09 lb	6.4E-09 kg
Solid Wastes		
Solid waste, process to landfill	24.7 lb	24.7 kg

Sources: Young, et. al. 2019, US EPA 2017a, US EPA 2015a, US EPA 2017b, API 2002, US EPA 2000

Table 15. Environmental Emissions for the Extraction of Crude Oil (Offshore Domestic)

	1,000 lb		**1,000 kg**	
Environmental Emissions				
Atmospheric Emissions				
Carbon dioxide	204	lb	204	kg
Carbon monoxide	0.61	lb	0.61	kg
Sulfur dioxide	0.027	lb	0.027	kg
Nitrogen oxides	0.71	lb	0.71	kg
Particulates, > 2.5 um, and < 10um	1.6E-05	lb	1.6E-05	kg
Particulates, < 2.5 um	0.0070	lb	0.0070	kg
VOC, volatile organic compounds	0.18	lb	0.18	kg
Waterborne Releases				
Chlorine	2.1E-07	lb	2.1E-07	kg
Solid Wastes				
Solid waste, process to landfill	24.7	lb	24.7	kg

Sources: Young, et. al. 2019, BOEM 2017, Cooney, et.al. 2017, US EPA 2015a, API 2002, US EPA 2000

Table 16. Environmental Emissions for the Extraction of Crude Oil (Onshore Foreign)

	1,000 lb		1,000 kg	
Environmental Emissions				
Atmospheric Emissions				
Carbon dioxide	438	lb	438	kg
Benzene, ethyl-	0.0023	lb	0.0023	kg
Styrene	1.5E-05	lb	1.5E-05	kg
Benzene, 1,4-dichloro-	2.2E-06	lb	2.2E-06	kg
Ethane, 1,2-dibromo-	1.3E-05	lb	1.3E-05	kg
Butadiene	4.7E-04	lb	4.7E-04	kg
Acrolein	0.0023	lb	0.0023	kg
Ethane, 1,2-dichloro-	6.0E-07	lb	6.0E-07	kg
Ethylene glycol	2.5E-08	lb	2.5E-08	kg
4-Methyl-2-pentanone	3.2E-06	lb	3.2E-06	kg
m-Xylene	4.8E-07	lb	4.8E-07	kg
Toluene	0.019	lb	0.019	kg
Benzene, chloro-	1.1E-05	lb	1.1E-05	kg
Phenol	5.8E-06	lb	5.8E-06	kg
Ethanol, 2-methoxy-	3.0E-07	lb	3.0E-07	kg
Hexane	0.0024	lb	0.0024	kg
Ethanol, 2-ethoxy-	9.0E-12	lb	9.0E-12	kg
Diethanolamine	1.2E-07	lb	1.2E-07	kg
Anthracene	3.8E-09	lb	3.8E-09	kg
1,4-Dioxane	1.3E-07	lb	1.3E-07	kg
Ethene, tetrachloro-	3.2E-06	lb	3.2E-06	kg
Pyrene	9.2E-09	lb	9.2E-09	kg
Hydrocarbons, aromatic	4.8E-06	lb	4.8E-06	kg
Cresol	1.6E-09	lb	1.6E-09	kg
Xylene	0.0049	lb	0.0049	kg
Chromium III	9.4E-07	lb	9.4E-07	kg
t-Butyl methyl ether	1.1E-10	lb	1.1E-10	kg
Glycol ethers	2.8E-08	lb	2.8E-08	kg
Arsenic, ion	1.6E-06	lb	1.6E-06	kg
Chromium VI	4.4E-07	lb	4.4E-07	kg
Benzo(g,h,i)perylene	2.1E-06	lb	2.1E-06	kg
Benzo(e)pyrene	1.6E-09	lb	1.6E-09	kg
Indeno(1,2,3-cd)pyrene	2.6E-10	lb	2.6E-10	kg
Perylene	1.9E-11	lb	1.9E-11	kg
Benzo(b)fluoranthene	1.1E-09	lb	1.1E-09	kg
Fluoranthene	9.5E-09	lb	9.5E-09	kg
Benzo(k)fluoranthene	1.9E-10	lb	1.9E-10	kg
Acenaphthylene	3.5E-08	lb	3.5E-08	kg
Chrysene	6.1E-09	lb	6.1E-09	kg
Hydrazine	5.0E-15	lb	5.0E-15	kg
Cyanamide	1.6E-09	lb	1.6E-09	kg
Carbonyl sulfide	1.6E-04	lb	1.6E-04	kg

Table 16. Environmental Emissions for the Extraction of Crude Oil (Onshore Foreign) (continued)

	1,000 lb	1,000 kg
Environmental Emissions		
Atmospheric Emissions		
Formaldehyde	0.022 lb	0.022 kg
Benzo(a)pyrene	2.0E-09 lb	2.0E-09 kg
Dibenz(a,h)anthracene	2.7E-10 lb	2.7E-10 kg
Pentane, 2,2,4-trimethyl-	2.1E-04 lb	2.1E-04 kg
Propene, 1,3-dichloro-	8.5E-06 lb	8.5E-06 kg
Methane, tetrachloro-, CFC-10	1.1E-05 lb	1.1E-05 kg
3-Methylcholanthrene	7.6E-11 lb	7.6E-11 kg
Benzo(a)anthracene	2.1E-07 lb	2.1E-07 kg
7,12-Dimethylbenz(a)anthracene	6.7E-10 lb	6.7E-10 kg
Carbon monoxide	0.81 lb	0.81 kg
Methanol	0.0026 lb	0.0026 kg
Chloroform	9.3E-06 lb	9.3E-06 kg
Benzene	0.031 lb	0.031 kg
Ethane, 1,1,1-trichloro-, HCFC-140	1.6E-05 lb	1.6E-05 kg
Lead	5.0E-06 lb	5.0E-06 kg
Manganese	6.1E-07 lb	6.1E-07 kg
Mercury	1.2E-07 lb	1.2E-07 kg
Nickel	5.5E-06 lb	5.5E-06 kg
Beryllium	4.7E-08 lb	4.7E-08 kg
Cadmium	1.7E-07 lb	1.7E-07 kg
Cobalt	6.1E-09 lb	6.1E-09 kg
Sulfur dioxide	0.10 lb	0.10 kg
Methane, bromo-, Halon 1001	1.4E-12 lb	1.4E-12 kg
Methane, monochloro-, R-40	5.4E-11 lb	5.4E-11 kg
Ethane, chloro-	1.0E-07 lb	1.0E-07 kg
Ethene, chloro-	5.6E-06 lb	5.6E-06 kg
Acetaldehyde	0.0026 lb	0.0026 kg
Methane, dichloro-, HCC-30	3.1E-05 lb	3.1E-05 kg
Carbon disulfide	8.2E-07 lb	8.2E-07 kg
Ethylene oxide	6.8E-11 lb	6.8E-11 kg
Ethane, 1,1-dichloro-	7.6E-06 lb	7.6E-06 kg
Ethene, 1,1-dichloro-	1.6E-09 lb	1.6E-09 kg
Propylene oxide	4.1E-07 lb	4.1E-07 kg
Hydrogen chloride	6.8E-07 lb	6.8E-07 kg
Ammonia	3.4E-04 lb	3.4E-04 kg
Phosphorus	1.1E-06 lb	1.1E-06 kg
Selenium	2.2E-07 lb	2.2E-07 kg
Chlorine	2.3E-07 lb	2.3E-07 kg
Hydrogen sulfide	5.5E-04 lb	5.5E-04 kg
Propane, 1,2-dichloro-	8.7E-06 lb	8.7E-06 kg

Table 16. Environmental Emissions for the Extraction of Crude Oil (Onshore Foreign) (continued)

	1,000 lb	1,000 kg
Environmental Emissions		
Atmospheric Emissions		
Ethane, 1,1,2-trichloro-	1.0E-05 lb	1.0E-05 kg
Ethene, trichloro-	6.1E-08 lb	6.1E-08 kg
Acrylamide	4.3E-11 lb	4.3E-11 kg
Ethane, 1,1,2,2-tetrachloro-	1.7E-05 lb	1.7E-05 kg
Acenaphthene	1.2E-08 lb	1.2E-08 kg
Phenanthrene	6.7E-08 lb	6.7E-08 kg
Fluorene	3.4E-08 lb	3.4E-08 kg
Naphthalene	6.9E-05 lb	6.9E-05 kg
Naphthalene, 2-methyl-	2.2E-07 lb	2.2E-07 kg
Biphenyl	1.2E-05 lb	1.2E-05 kg
o-Xylene	1.0E-07 lb	1.0E-07 kg
Cumene	1.9E-08 lb	1.9E-08 kg
Acetophenone	1.1E-09 lb	1.1E-09 kg
Nitrogen oxides	0.58 lb	0.58 kg
Particulates, > 2.5 um, and < 10um	4.1E-04 lb	4.1E-04 kg
Particulates, < 2.5 um	0.017 lb	0.017 kg
VOC, volatile organic compounds	5.59 lb	5.59 kg
Waterborne Releases		
Dissolved solids	0.027 lb	0.027 kg
Suspended solids, unspecified	0.0067 lb	0.0067 kg
Sulfate	0.010 lb	0.010 kg
Chloride	0.0016 lb	0.0016 kg
Hydrocarbons, aromatic	1.9E-04 lb	1.9E-04 kg
Ammonia	4.8E-05 lb	4.8E-05 kg
Manganese	3.5E-05 lb	3.5E-05 kg
Oils, unspecified	3.3E-05 lb	3.3E-05 kg
Fluoride	4.3E-06 lb	4.3E-06 kg
Bromide	2.1E-07 lb	2.1E-07 kg
Copper	5.6E-08 lb	5.6E-08 kg
Chlorine	6.5E-10 lb	6.5E-10 kg
Zinc	1.9E-08 lb	1.9E-08 kg
Benzene, ethyl-	7.6E-10 lb	7.6E-10 kg
Mercury	8.3E-11 lb	8.3E-11 kg
Radium-226	3.9E-21 Cu	1.5E-13 kBq
Sulfide	7.2E-05 lb	7.2E-05 kg
Toluene	5.2E-09 lb	5.2E-09 kg
Xylene	6.4E-09 lb	6.4E-09 kg
Solid Wastes		
Solid waste, process to landfill	24.7 lb	24.7 kg

Sources: Young, et.al. 2019, Cooney, et.al. 2017, US EIA 2017b, Schlanger 2016, US EPA 2015a, API 2002, US EPA 2000

Table 17. Environmental Emissions for the Extraction of Crude Oil (Offshore Foreign)

	1,000 lb	1,000 kg
Environmental Emissions		
Atmospheric Emissions		
Carbon dioxide	204 lb	204 kg
Carbon monoxide	0.61 lb	0.61 kg
Sulfur dioxide	0.027 lb	0.027 kg
Nitrogen oxides	0.71 lb	0.71 kg
Particulates, > 2.5 um, and < 10um	1.6E-05 lb	1.6E-05 kg
Particulates, < 2.5 um	0.0070 lb	0.0070 kg
VOC, volatile organic compounds	0.18 lb	0.18 kg
Waterborne Releases		
Chlorine	2.1E-07 lb	2.1E-07 kg
Solid Wastes		
Solid waste, process to landfill	24.7 lb	24.7 kg

Sources: Young, et.al. 2019, Cooney, et.al. 2017, US EIA 2017b, Schlanger 2016, US EPA 2015a, API 2002, US EPA 2000

PETROLEUM REFINING

The refining process begins in a distilling column, where liquid oil is heated to a vapor and lifted upward to be distilled again into separate substances. Distilling exploits the characteristic of the chemicals in crude oil to boil at different temperatures, a phenomenon that engineers chart along distillation curves. A distilling column contains a set of trays that allow heated vapors to rise and collect at different levels, separating out the various liquids derived from crude oil. Since the top of the column is cooler than the bottom, the liquids vaporize and rise, then they condense again, collecting onto their respective trays. Butane and other light products rise to the top of the column, while straight-run gasoline, naphtha, kerosene, diesel, and heavy gas oil gather on the trays, leaving straight run residue at the base of the column. Liquids are considered “heavy” or “light” based on their specific gravity, which is determined based on its weight and density compared to that of water.

Because there is more demand for some distilled products like gasoline, refiners have an incentive to convert heavy liquids into lighter liquids. The term cracking comes from the process of breaking up long hydrocarbon molecules into smaller, more useful molecules. The cracking process converts heavy straight run liquids into lighter liquids, such as gasoline. There are multiple versions of the cracking process, and refiners use the process extensively. Cracking is a highly controlled process, so cracking units exist separate from distillation columns. The most common type of cracking is “cat cracking,” named for the use of catalysts, substances added to a chemical reaction to speed up the process. The products from the cracking process may then go to a reformer to create gasoline or other fuels. For this analysis, no further processes are considered beyond the cracker as naphtha is the common refinery feed sent to steam crackers (olefins plants).

The refinery process key inputs include crude petroleum, electricity, and natural gas. Key outputs include refinery products and emissions to air, water, and soil. The emission data for the process is adapted from inventory data compiled by the National Energy Technology Lab. The following briefly summarizes that data collection effort as documented in [Young, et. al, 2019]. Reported emissions from petroleum refineries in 2014 were compiled from EPA datasets including NEI, DMR, Toxic Release Inventory (TRI) and the Greenhouse Gas Reporting Program (GHGRP). Emissions data, representing releases to air, water, and soil covers 153 U.S. refineries. Crude oil consumption was calculated based on reported operating capacities by refinery and reported utilization (US EIA, 2016). Total production of U.S. refining products is reported by the Energy Information Administration (US EIA, 2017a). EIA also reports annual fuel and material consumption by region (US EIA, 2017n, US EIA, 2017o).

Water consumption data was documented in [Wu, M. et. al., 2009]. The amount used here is an average with the range given as 0.55 to 2.75 cubic meters per 1,000 kg of refined oil. The lower amounts are inclined to come from newer refineries.

No new sources were found for solid wastes created at a refinery. The previous source (Oak Ridge, 1996) was used, which provides the solid waste on a basis of crude oil input. The amount of crude oil required to produce 1,000 kg of refined oil was updated in the calculation.

Data for transport distances of crude oil to the refinery are sourced from Young et. al. 2019. EIA reports annual crude imports by country of origin. Travel distances from those countries via ship were estimated with a shipping distance calculator (Sea-Distances.org). Internal domestic transport of crude oil within and between PADDs by transport type is reported by EIA (US EIA 2017k, US EIA 2017l).

Table 18 provides the LCI input and output data for 1,000 pounds and 1,000 kilograms of refined oil.

Table 18. LCI Data for the Refining of Petroleum Products

	1,000 lb		1,000 kg	
Material Inputs				
Hydrogen gas	4.59	lb	4.59	kg
Methyl tert-butyl	0.14	lb	0.14	kg
Ethanol	3.18	lb	3.18	kg
Sulfuric acid	1.39	lb	1.39	kg
Hydrogen fluoride	0.0042	lb	0.0042	kg
Crude oil	954	lb	954	kg
Energy				
Process Energy				
Electricity from grid	24.9	kWh	54.8	kWh
Natural gas	73.5	ft^3	4.59	m^3
Coal	0.018	lb	0.018	kg
Liquid petroleum gas (LPG)	4.05	gal	0.034	m^3
Residual oil	0.0046	gal	3.9E-05	m^3
Transportation Energy				
Barge	4.97	ton·mi	16.0	tonne·km
Ship	962	ton·mi	3,098	tonne·km
Petroleum Pipeline	183	ton·mi	588	tonne·km
Rail	45.0	ton·mi	145	tonne·km
Environmental Emissions				
Atmospheric Emissions				
Carbon monoxide	0.061	lb	0.061	kg
Nitrogen oxides	0.092	lb	0.092	kg
Particulates, > 2.5 um, and < 10um	0.0035	lb	0.0035	kg
Particulates, < 2.5 um	0.022	lb	0.022	kg
Sulfur dioxide	0.039	lb	0.039	kg
VOC, volatile organic compounds	0.070	lb	0.070	kg
Ethane, 1,1,1-trichloro-, HCFC-140	9.1E-07	lb	9.1E-07	kg
Ethane, 1,1,2,2-tetrachloro-	3.1E-08	lb	3.1E-08	kg
Benzidine, 3,3'-dimethoxy-	6.3E-08	lb	6.3E-08	kg
Benzene, 1,2,4-trichloro-	9.1E-09	lb	9.1E-09	kg
Butane, 1,2-epoxy-	1.7E-07	lb	1.7E-07	kg
Benzene, 1,4-dichloro-	2.4E-08	lb	2.4E-08	kg
1,4-Dioxane	1.2E-08	lb	1.2E-08	kg
1-Methylnapthalene	1.7E-07	lb	1.7E-07	kg
Pentane, 2,2,4-trimethyl-	1.8E-04	lb	1.8E-04	kg
Phenol, 2,4,5-trichloro-	9.1E-09	lb	9.1E-09	kg
Phenol, 2,4,6-trichloro-	1.0E-08	lb	1.0E-08	kg
Phenol, 2,4-dinitro-	9.1E-09	lb	9.1E-09	kg

Table 18. LCI Data for the Refining of Petroleum Products (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
Atmospheric Emissions				
Ethanol, 2-methoxy-	2.5E-07	lb	2.5E-07	kg
Naphthalene, 2-methyl-	2.8E-07	lb	2.8E-07	kg
Propane, 2-nitro-	8.6E-08	lb	8.6E-08	kg
Benzidine, 3,3'-dichloro-	9.1E-09	lb	9.1E-09	kg
Benzidine, 3,3'-dimethyl-	4.4E-08	lb	4.4E-08	kg
3-Methylcholanthrene	2.9E-11	lb	2.9E-11	kg
4,4'-Methylenebisbenzeneamine	2.7E-08	lb	2.7E-08	kg
Phenol, 4-nitro-	9.1E-09	lb	9.1E-09	kg
Phenanthrene	1.0E-08	lb	1.0E-08	kg
Acenaphthene	1.8E-09	lb	1.8E-09	kg
Acenaphthylene	2.6E-09	lb	2.6E-09	kg
Acetaldehyde	2.6E-05	lb	2.6E-05	kg
Acetamide	8.5E-10	lb	8.5E-10	kg
Acetonitrile	7.5E-06	lb	7.5E-06	kg
Acetophenone	6.1E-07	lb	6.1E-07	kg
Acrolein	6.4E-06	lb	6.4E-06	kg
Acrylonitrile	2.0E-08	lb	2.0E-08	kg
Ammonia	0.0033	lb	0.0033	kg
Aniline	9.2E-07	lb	9.2E-07	kg
Anthracene	4.1E-08	lb	4.1E-08	kg
Antimony	6.7E-06	lb	6.7E-06	kg
Arsenic, ion	5.7E-07	lb	5.7E-07	kg
Asbestos	7.5E-10	lb	7.5E-10	kg
Benzo(a)anthracene	6.3E-08	lb	6.3E-08	kg
Benzene	6.4E-04	lb	6.4E-04	kg
Benzene, chloro-	3.5E-07	lb	3.5E-07	kg
Benzene, ethyl-	2.0E-04	lb	2.0E-04	kg
Benzidine	9.7E-08	lb	9.7E-08	kg
Benzo(a)pyrene	1.1E-05	lb	1.1E-05	kg
Benzo(b)fluoranthene	4.4E-09	lb	4.4E-09	kg
Benzo(e)pyrene	5.0E-11	lb	5.0E-11	kg
Benzo(g,h,i)perylene	1.6E-06	lb	1.6E-06	kg
Benzo(k)fluoranthene	1.1E-09	lb	1.1E-09	kg
Benzofluoranthene	5.1E-09	lb	5.1E-09	kg
Beryllium	5.9E-08	lb	5.9E-08	kg
Biphenyl	9.4E-06	lb	9.4E-06	kg
Bis(2-chloroethyl)ether	9.1E-09	lb	9.1E-09	kg
Butadiene	6.1E-05	lb	6.1E-05	kg

Table 18. LCI Data for the Refining of Petroleum Products (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
Atmospheric Emissions				
Cadmium	7.7E-07	lb	7.7E-07	kg
Carbon disulfide	4.0E-05	lb	4.0E-05	kg
Methane, tetrachloro-, CFC-10	4.4E-07	lb	4.4E-07	kg
Carbonyl sulfide	2.0E-04	lb	2.0E-04	kg
Catechol	1.2E-07	lb	1.2E-07	kg
Chlorine	3.9E-05	lb	3.9E-05	kg
Chloroform	5.1E-06	lb	5.1E-06	kg
Naphthalene, beta-chloro-	6.4E-14	lb	6.4E-14	kg
Chromium VI	4.8E-07	lb	4.8E-07	kg
Chromium III	2.8E-06	lb	2.8E-06	kg
Chrysene	9.0E-08	lb	9.0E-08	kg
Tar	1.7E-07	lb	1.7E-07	kg
Cobalt	6.1E-07	lb	6.1E-07	kg
Cresol	2.5E-05	lb	2.5E-05	kg
Cumene	1.1E-04	lb	1.1E-04	kg
Cyanamide	7.0E-04	lb	7.0E-04	kg
Dibenz(a,h)anthracene	1.2E-08	lb	1.2E-08	kg
Benz(a)acridine	7.2E-11	lb	7.2E-11	kg
Benzo(e)pyrene	1.9E-09	lb	1.9E-09	kg
Dibenzofuran	2.8E-08	lb	2.8E-08	kg
Diethanolamine	5.5E-05	lb	5.5E-05	kg
Dimethyl formamide	3.7E-09	lb	3.7E-09	kg
4-Dimethylaminoazobenzene	5.2E-09	lb	5.2E-09	kg
Epichlorohydrin	6.5E-06	lb	6.5E-06	kg
Ethane, 1,1,2-trichloro-	9.2E-09	lb	9.2E-09	kg
Ethane, 1,1-dichloro-	5.0E-09	lb	5.0E-09	kg
Ethane, 1,2-dibromo-	2.7E-06	lb	2.7E-06	kg
Ethane, 1,2-dichloro-	1.1E-06	lb	1.1E-06	kg
Ethene, chloro-	3.8E-09	lb	3.8E-09	kg
Ethene, tetrachloro-	2.4E-05	lb	2.4E-05	kg
Ethylene glycol	1.5E-05	lb	1.5E-05	kg
Fluoranthene	6.9E-07	lb	6.9E-07	kg
Fluorene	1.2E-08	lb	1.2E-08	kg
Formaldehyde	3.5E-04	lb	3.5E-04	kg
Glycol ethers	1.1E-05	lb	1.1E-05	kg
Butadiene, hexachloro-	9.1E-09	lb	9.1E-09	kg
Benzene, hexachloro-	9.1E-09	lb	9.1E-09	kg

Table 18. LCI Data for the Refining of Petroleum Products (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
Atmospheric Emissions				
Cyclopentadiene, hexachloro-	9.1E-09	lb	9.1E-09	kg
Ethane, hexachloro-	9.1E-09	lb	9.1E-09	kg
Hexane, 1,6-diisocyanato-	5.2E-08	lb	5.2E-08	kg
Hexane	0.0013	lb	0.0013	kg
Hydrazine	4.3E-10	lb	4.3E-10	kg
Hydrocarbons, aromatic	1.2E-05	lb	1.2E-05	kg
Hydrogen chloride	2.4E-04	lb	2.4E-04	kg
Hydrogen cyanide	0.0022	lb	0.0022	kg
Hydrogen fluoride	2.8E-05	lb	2.8E-05	kg
Hydrogen sulfide	7.3E-04	lb	7.3E-04	kg
Indeno(1,2,3-cd)pyrene	1.5E-08	lb	1.5E-08	kg
Isophorone	1.3E-08	lb	1.3E-08	kg
Lead	2.3E-06	lb	2.3E-06	kg
Manganese	5.4E-06	lb	5.4E-06	kg
m-Cresol	3.8E-08	lb	3.8E-08	kg
Mercury	7.9E-07	lb	7.9E-07	kg
Methane, bromo-, Halon 1001	3.7E-06	lb	3.7E-06	kg
Methane, dichloro-, HCC-30	1.8E-05	lb	1.8E-05	kg
Methane, monochloro-, R-40	5.0E-08	lb	5.0E-08	kg
Methanol	5.6E-04	lb	5.6E-04	kg
4-Methyl-2-pentanone	2.0E-04	lb	2.0E-04	kg
4,4'-Diisocyanatodiphenylmethane	8.0E-08	lb	8.0E-08	kg
Ethane, chloro-	1.8E-10	lb	1.8E-10	kg
Diisobutyl ketone	4.0E-06	lb	4.0E-06	kg
Naphthalene	1.4E-04	lb	1.4E-04	kg
Nickel	1.6E-05	lb	1.6E-05	kg
Nickel refinery dust	2.1E-11	lb	2.1E-11	kg
Nitrobenzene	1.7E-07	lb	1.7E-07	kg
N-Nitrosodimethylamine	9.1E-09	lb	9.1E-09	kg
o-Cresol	3.5E-13	lb	3.5E-13	kg
o-Toluidine	1.8E-08	lb	1.8E-08	kg
o-Xylene	6.0E-07	lb	6.0E-07	kg
p-Xylene	4.8E-07	lb	4.8E-07	kg
Phenol, pentachloro-	2.0E-08	lb	2.0E-08	kg
Perylene	5.8E-12	lb	5.8E-12	kg
Phenanthrene	7.5E-06	lb	7.5E-06	kg
Phenol	8.2E-05	lb	8.2E-05	kg
Phosphorus	1.1E-06	lb	1.1E-06	kg
Phthalate, dibutyl-	2.6E-07	lb	2.6E-07	kg

Table 18. LCI Data for the Refining of Petroleum Products (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
Atmospheric Emissions				
Phthalate, dimethyl-	9.1E-09	lb	9.1E-09	kg
Phthalate, dioctyl-	3.4E-07	lb	3.4E-07	kg
Polychlorinated biphenyls	5.7E-12	lb	5.7E-12	kg
p-Phenylenediamine	3.9E-08	lb	3.9E-08	kg
Propanal	9.3E-09	lb	9.3E-09	kg
Propane, 1,2-dichloro-	5.9E-09	lb	5.9E-09	kg
Propene, 1,3-dichloro-	1.2E-08	lb	1.2E-08	kg
Ethanol, 2-propoxy-	4.5E-08	lb	4.5E-08	kg
Propylene oxide	3.4E-08	lb	3.4E-08	kg
Pyrene	9.1E-07	lb	9.1E-07	kg
Quinoline	1.7E-08	lb	1.7E-08	kg
Selenium	5.8E-07	lb	5.8E-07	kg
Styrene	1.3E-05	lb	1.3E-05	kg
t-Butyl methyl ether	3.1E-05	lb	3.1E-05	kg
Toluene	0.0011	lb	0.0011	kg
Toluene, 2,4-dinitro-	9.1E-09	lb	9.1E-09	kg
Ethene, trichloro-	5.2E-06	lb	5.2E-06	kg
Vinyl acetate	8.3E-08	lb	8.3E-08	kg
Xylene	9.0E-04	lb	9.0E-04	kg
Dioxin, 1,2,3,4,6,7,8,9-octachlorodibenzo-p-	2.2E-12	lb	2.2E-12	kg
Dibenzofuran, 1,2,3,4,6,7,8,9-octachloro-	1.6E-12	lb	1.6E-12	kg
Dioxin, 1,2,3,4,6,7,8-heptachlorodibenzo-p-	1.5E-12	lb	1.5E-12	kg
Dibenzofuran, 1,2,3,4,6,7,8-heptachloro-	5.5E-12	lb	5.5E-12	kg
1,2,3,4,7,8,9 Heptachlorodibenzofuran	1.3E-12	lb	1.3E-12	kg
Dioxin, 1,2,3,4,7,8-hexachlorodibenzo-p	3.3E-13	lb	3.3E-13	kg
Dibenzofuran, 1,2,3,4,7,8-hexachloro-	1.9E-12	lb	1.9E-12	kg
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	4.9E-13	lb	4.9E-13	kg
Dibenzofuran, 1,2,3,6,7,8-hexachloro-	2.0E-12	lb	2.0E-12	kg
Dioxin, 1,2,3,7,8,9-hexachlorodibenzo-	4.1E-13	lb	4.1E-13	kg
Dibenzofuran, 1,2,3,7,8,9-hexachloro-	1.2E-12	lb	1.2E-12	kg
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	3.2E-13	lb	3.2E-13	kg
Dibenzofuran, 1,2,3,7,8-pentachloro-	1.4E-12	lb	1.4E-12	kg
Benzene, 1,2,4-trimethyl-	2.1E-04	lb	2.1E-04	kg
1-Methyl-2-pyrrolidinone	3.9E-06	lb	3.9E-06	kg
Dibenzofuran, 2,3,4,6,7,8-hexachloro-	1.9E-12	lb	1.9E-12	kg
Dibenzofuran, 2,3,4,7,8-pentachloro-	1.7E-12	lb	1.7E-12	kg
Dioxin, 2,3,7,8 Tetrachlorodibenzo-p-	4.0E-13	lb	4.0E-13	kg
Dibenzofuran, 2,3,7,8-tetrachloro-	1.2E-12	lb	1.2E-12	kg

Table 18. LCI Data for the Refining of Petroleum Products (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
Atmospheric Emissions				
Phenol, 2,4-dimethyl-	1.8E-07	lb	1.8E-07	kg
Bisphenol A	5.6E-06	lb	5.6E-06	kg
Barium	4.3E-09	lb	4.3E-09	kg
Barium compounds	1.9E-07	lb	1.9E-07	kg
1-Butanol	7.4E-07	lb	7.4E-07	kg
Copper	2.3E-07	lb	2.3E-07	kg
Copper compounds	1.2E-06	lb	1.2E-06	kg
4-Methyl-2-methoxyphenol	3.1E-08	lb	3.1E-08	kg
Cyclohexane	2.8E-04	lb	2.8E-04	kg
Dicyclopentadiene	1.7E-06	lb	1.7E-06	kg
Ethene	6.1E-04	lb	6.1E-04	kg
Isoprene	4.8E-06	lb	4.8E-06	kg
Methane, chlorodifluoro-, HCFC-22	1.1E-05	lb	1.1E-05	kg
Molybdenum trioxide	1.2E-06	lb	1.2E-06	kg
Glycidol	3.5E-08	lb	3.5E-08	kg
Ozone	3.7E-05	lb	3.7E-05	kg
Propene	0.0010	lb	0.0010	kg
Silver compounds	6.0E-06	lb	6.0E-06	kg
Sulfuric acid	0.0024	lb	0.0024	kg
t-Butyl alcohol	2.0E-07	lb	2.0E-07	kg
Vanadium	1.1E-08	lb	1.1E-08	kg
Vanadium compounds	2.3E-06	lb	2.3E-06	kg
Zinc compounds	2.8E-05	lb	2.8E-05	kg
Carbon dioxide	220	lb	220	kg
Methane	0.036	lb	0.036	kg
Nitrous oxide	0.0019	lb	0.0019	kg
Waterborne emissions				
Dibenzofuran, 1,2,3,4,6,7,8-heptachloro-	4.1E-13	lb	4.1E-13	kg
Dibenzofuran, 1,2,3,4,7,8-hexachloro-	3.3E-13	lb	3.3E-13	kg
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	5.1E-14	lb	5.1E-14	kg
Dioxin, 1,2,3,7,8,9-hexachlorodibenzo-	4.8E-14	lb	4.8E-14	kg
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	4.0E-14	lb	4.0E-14	kg
Benzene, 1,2,4-trimethyl-	6.9E-07	lb	6.9E-07	kg
1-Methyl-2-pyrrolidinone	1.5E-08	lb	1.5E-08	kg
Dibenzofuran, 2,3,4,6,7,8-hexachloro-	5.3E-14	lb	5.3E-14	kg
Dibenzofuran, 2,3,4,7,8-pentachloro-	7.7E-14	lb	7.7E-14	kg
Dioxin, 2,3,7,8 Tetrachlorodibenzo-p-	1.7E-14	lb	1.7E-14	kg
Dibenzofuran, 2,3,7,8-tetrachloro-	3.5E-14	lb	3.5E-14	kg
Phenol, 2,4-dimethyl-	1.5E-07	lb	1.5E-07	kg
Acetonitrile	3.8E-07	lb	3.8E-07	kg

Table 18. LCI Data for the Refining of Petroleum Products (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
Waterborne emissions				
Ammonia	2.0E-04	lb	2.0E-04	kg
Anthracene	6.5E-08	lb	6.5E-08	kg
Antimony compounds	2.2E-06	lb	2.2E-06	kg
Barium compounds	2.9E-06	lb	2.9E-06	kg
Benzene, ethyl-	9.8E-07	lb	9.8E-07	kg
Benzo(g,h,i)perylene	8.8E-08	lb	8.8E-08	kg
Butadiene	5.3E-08	lb	5.3E-08	kg
Cadmium compounds	1.1E-09	lb	1.1E-09	kg
Carbon disulfide	1.1E-06	lb	1.1E-06	kg
Chlorine	2.5E-07	lb	2.5E-07	kg
Chromium	3.5E-07	lb	3.5E-07	kg
Chromium compounds	2.5E-07	lb	2.5E-07	kg
Cobalt compounds	6.7E-07	lb	6.7E-07	kg
Copper	1.4E-07	lb	1.4E-07	kg
Copper compounds	3.9E-07	lb	3.9E-07	kg
Cresol	1.0E-06	lb	1.0E-06	kg
Cumene	4.1E-07	lb	4.1E-07	kg
Cyanamide	4.3E-07	lb	4.3E-07	kg
Cyclohexane	3.7E-07	lb	3.7E-07	kg
Diethanolamine	5.8E-07	lb	5.8E-07	kg
Ethene	3.5E-07	lb	3.5E-07	kg
Ethene, tetrachloro-	7.9E-08	lb	7.9E-08	kg
Ethylene glycol	2.5E-05	lb	2.5E-05	kg
Ethanol, 2-ethoxy-	2.1E-07	lb	2.1E-07	kg
Hexane	7.4E-07	lb	7.4E-07	kg
Hydrogen fluoride	6.0E-09	lb	6.0E-09	kg
Hydrogen sulfide	1.3E-05	lb	1.3E-05	kg
Isoprene	5.4E-07	lb	5.4E-07	kg
Lead	1.6E-08	lb	1.6E-08	kg
Lead compounds	1.1E-06	lb	1.1E-06	kg
Manganese	4.1E-06	lb	4.1E-06	kg
Manganese compounds	9.3E-07	lb	9.3E-07	kg
Mercury	1.4E-09	lb	1.4E-09	kg
Mercury compounds	4.2E-08	lb	4.2E-08	kg
Methanol	3.7E-05	lb	3.7E-05	kg
4-Methyl-2-pentanone	2.3E-08	lb	2.3E-08	kg
Molybdenum trioxide	2.2E-06	lb	2.2E-06	kg
m-Xylene	2.1E-08	lb	2.1E-08	kg

Table 18. LCI Data for the Refining of Petroleum Products (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
Waterborne emissions				
Naphthalene	1.0E-06	lb	1.0E-06	kg
Nickel	4.6E-08	lb	4.6E-08	kg
Nickel compounds	5.5E-06	lb	5.5E-06	kg
Nitrate compounds	1.2E-02	lb	1.2E-02	kg
o-Xylene	2.1E-07	lb	2.1E-07	kg
PAH, polycyclic aromatic hydrocarbons	6.5E-07	lb	6.5E-07	kg
p-Xylene	2.0E-08	lb	2.0E-08	kg
Phenanthrene	9.2E-08	lb	9.2E-08	kg
Phenol	5.5E-06	lb	5.5E-06	kg
Propene	3.7E-07	lb	3.7E-07	kg
Selenium	6.4E-07	lb	6.4E-07	kg
Selenium compounds	1.8E-06	lb	1.8E-06	kg
Silver compounds	5.4E-12	lb	5.4E-12	kg
Styrene	3.9E-07	lb	3.9E-07	kg
t-Butyl methyl ether	5.4E-10	lb	5.4E-10	kg
t-Butyl alcohol	6.5E-09	lb	6.5E-09	kg
Toluene	2.5E-06	lb	2.5E-06	kg
Vanadium compounds	1.7E-05	lb	1.7E-05	kg
Xylene	5.1E-06	lb	5.1E-06	kg
Zinc compounds	2.7E-05	lb	2.7E-05	kg
Naphthalene, 2-methyl-	2.2E-08	lb	2.2E-08	kg
Acenaphthene	7.6E-10	lb	7.6E-10	kg
Acenaphthylene	7.6E-10	lb	7.6E-10	kg
Benzo(a)anthracene	3.1E-08	lb	3.1E-08	kg
Benzo(a)pyrene	3.1E-08	lb	3.1E-08	kg
Benzo(k)fluoranthene	7.6E-10	lb	7.6E-10	kg
BOD5, Biological Oxygen Demand	1.1E-02	lb	1.1E-02	kg
Chromium VI	7.6E-07	lb	7.6E-07	kg
Chromium III	2.8E-07	lb	2.8E-07	kg
Chrysene	1.8E-08	lb	1.8E-08	kg
COD, Chemical Oxygen Demand	2.7E-02	lb	2.7E-02	kg
Dibenz(a,h)anthracene	1.8E-08	lb	1.8E-08	kg
Fluorene	7.6E-10	lb	7.6E-10	kg
PAH, polycyclic aromatic hydrocarbons	9.3E-16	lb	9.3E-16	kg
Nitrogen, total	4.3E-04	lb	4.3E-04	kg
Oils, unspecified	1.5E-03	lb	1.5E-03	kg
Pyrene	1.8E-08	lb	1.8E-08	kg
Silver	6.5E-10	lb	6.5E-10	kg

Table 18. LCI Data for the Refining of Petroleum Products (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
Waterborne Emissions				
Dissolved solids	1.9E-01	lb	1.9E-01	kg
Suspended solids, unspecified	1.7E-02	lb	1.7E-02	kg
Sulfur	1.9E-08	lb	1.9E-08	kg
TOC, Total Organic Carbon	7.1E-03	lb	7.1E-03	kg
Soil Emissions				
Benzene, 1,2,4-trimethyl-	2.6E-06	lb	2.6E-06	kg
Aluminium oxide, fibrous forms	2.4E-04	lb	2.4E-04	kg
Ammonia	1.4E-06	lb	1.4E-06	kg
Anthracene	1.3E-08	lb	1.3E-08	kg
Barium compounds	3.6E-11	lb	3.6E-11	kg
Benzene	1.4E-06	lb	1.4E-06	kg
Benzene, ethyl-	7.9E-07	lb	7.9E-07	kg
Benzo(g,h,i)perylene	3.0E-07	lb	3.0E-07	kg
Biphenyl	1.1E-08	lb	1.1E-08	kg
Butadiene	3.3E-09	lb	3.3E-09	kg
Cadmium compounds	4.9E-09	lb	4.9E-09	kg
Chromium	5.4E-10	lb	5.4E-10	kg
Chromium compounds	5.2E-07	lb	5.2E-07	kg
Cobalt compounds	6.1E-07	lb	6.1E-07	kg
Copper compounds	8.3E-07	lb	8.3E-07	kg
4-Methyl-2-methoxyphenol	1.8E-07	lb	1.8E-07	kg
Cresol	8.0E-08	lb	8.0E-08	kg
Cumene	2.1E-07	lb	2.1E-07	kg
Cyanide compounds	5.3E-08	lb	5.3E-08	kg
Cyclohexane	1.5E-07	lb	1.5E-07	kg
Dibenzofuran	3.4E-10	lb	3.4E-10	kg
Ethane, 1,2-dibromo-	1.3E-11	lb	1.3E-11	kg
Ethene	2.6E-08	lb	2.6E-08	kg
Ethene, tetrachloro-	6.9E-10	lb	6.9E-10	kg
Hexane	1.9E-06	lb	1.9E-06	kg
Hydrogen fluoride	7.1E-10	lb	7.1E-10	kg
Hydrogen sulfide	2.2E-07	lb	2.2E-07	kg
Isoprene	1.1E-09	lb	1.1E-09	kg
Lead	3.0E-09	lb	3.0E-09	kg
Lead compounds	2.7E-06	lb	2.7E-06	kg
Manganese	2.0E-08	lb	2.0E-08	kg
Manganese compounds	4.8E-07	lb	4.8E-07	kg

Table 18. LCI Data for the Refining of Petroleum Products (continued)

	1,000 lb		1,000 kg	
Environmental Emissions				
Soil Emissions				
Mercury	8.5E-09	lb	8.5E-09	kg
Mercury compounds	8.0E-08	lb	8.0E-08	kg
Molybdenum trioxide	5.6E-06	lb	5.6E-06	kg
m-Xylene	7.8E-07	lb	7.8E-07	kg
Naphthalene	9.7E-07	lb	9.7E-07	kg
Nickel	1.6E-07	lb	1.6E-07	kg
Nickel compounds	1.7E-05	lb	1.7E-05	kg
Nitrate compounds	5.4E-05	lb	5.4E-05	kg
o-Xylene	5.4E-08	lb	5.4E-08	kg
PAH, polycyclic aromatic hydrocarbons	2.5E-06	lb	2.5E-06	kg
p-Xylene	2.1E-08	lb	2.1E-08	kg
Phenanthrene	3.8E-07	lb	3.8E-07	kg
Phenol	3.6E-08	lb	3.6E-08	kg
Propene	6.4E-08	lb	6.4E-08	kg
Selenium compounds	6.4E-11	lb	6.4E-11	kg
Styrene	8.3E-08	lb	8.3E-08	kg
Toluene	1.7E-06	lb	1.7E-06	kg
Vanadium compounds	1.6E-05	lb	1.6E-05	kg
Xylene	1.5E-05	lb	1.5E-05	kg
Zinc compounds	5.5E-06	lb	5.5E-06	kg
Solid Wastes				
Solid waste, process to landfill	5.17	lb	5.17	kg
Water Consumption	201	gal	1.68	m^3

Sources: Young, et. al. 2019, NETL, 2017b and Oak Ridge, 1996.

NATURAL GAS PRODUCTION

Natural gas is extracted from deep underground wells and is frequently co-produced with crude oil. Because of its gaseous nature, natural gas flows quite freely from wells which produce primarily natural gas, but some energy is required to pump natural gas and crude oil mixtures to the surface. The principal composition of all natural gas is methane (CH4), other components of natural gas include ethane, propane, butane, and other heavier hydrocarbons, as well as water vapor, carbon dioxide, nitrogen, and hydrogen sulfides.

Atmospheric emissions from natural gas production result primarily from unflared venting. Methane and non-combustion carbon dioxide emissions from natural gas extraction are generally process-related, with the largest source of these emissions from normal operations, system upsets, and routine maintenance. Waterborne wastes result from brines that occur when natural gas is produced in combination with oil and from produced water production from hydraulic fracturing.

There are two types of natural gas extraction processes, conventional resource extraction and unconventional resource extraction. Conventional resources are concentrations of natural gas that occur in discrete accumulations or pools. Rock formations hosting these pools traditionally have high porosity and permeability and are found below impermeable rock formations. These impervious layers form barriers to hydrocarbon migration resulting in oil and gas being trapped below them. Conventional natural gas pools are developed using vertical well bores and using minimal stimulation. Unconventional resources are natural gas-bearing units where the permeability and porosity are so low that the resource cannot be extracted economically through a vertical well bore and instead requires a horizontal well bore followed by multistage hydraulic fracturing to achieve economic production.

The term of conventional extraction applies to oil and gas which can be extracted, after the drilling operations, just by the natural pressure of the wells and pumping or compression operations. After the depletion of maturing fields, the natural pressure of the wells may be too low to produce significant quantities of oil and gas. Different techniques may be used to boost production, mainly water and gas injection or depletion compression, which are still considered conventional extraction.

Hydraulic fracturing is a technique used in "unconventional" gas production. "Unconventional" reservoirs can cost-effectively produce gas only by using a special stimulation technique, like hydraulic fracturing, or other special recovery process and technology. This is often because the gas is highly dispersed in the rock, rather than occurring in a concentrated underground location (US EPA, 2018).

Extracting unconventional gas is relatively new. Coalbed methane production began in the 1980s; shale gas extraction is even more recent. The main enabling technologies, hydraulic fracturing and horizontal drilling, have opened up new areas for oil and gas development, with particular focus on natural gas reservoirs such as shale, coalbed and tight sands.

Natural gas may also be identified as dry or wet. Wet natural gas is rich in liquid hydrocarbons, such as oil and NGL. Dry natural gas is natural gas that remains after the liquefiable hydrocarbon portion has been removed from the gas stream (i.e., gas after lease, field, and/or plant separation), and any volumes of non-hydrocarbon gases have been removed where they occur in sufficient quantity to render the gas unmarketable (US DOE, 2015).

This unit process encompasses the material outputs for the extraction of natural gas from both conventional and unconventional sources. The inputs to this unit process are natural gas, ground water, and surface water. These three inputs are natural resources and thus enter the boundary of this unit process with no upstream environmental burdens. If the natural gas extraction site is near a source of electricity, it is financially preferable to use electrically powered equipment instead of gas-powered equipment. This is the case for extraction sites for Barnett and Marcellus Shale. The output is dehydrated natural gas that is suitable for pipeline transport and subsequent processing steps such as sweetening or, in the case of imported natural gas, liquefaction.

In 2016, an estimated 40 percent of natural gas came from conventional onshore and offshore sources including associated onshore natural gas production and an estimated 60 percent of natural gas was sourced from unconventional natural gas resources including shale well and CBM extraction (US EIA, 2017b). Natural gas extraction is characterized by six types of extraction, namely onshore conventional, offshore conventional, associated natural gas, Barnett Shale, Marcellus Shale, and coalbed methane natural gas. The natural gas extraction data set is a mix of the extraction types shown as percentages in Table 19. The input and output data for each of the subprocesses is taken from NETL unit process library with the most recent data from 2010. A brief explanation of each extraction method is provided and detailed LCI data provided in the tables that follow.

Table 19. Percentage Contribution by Type of Natural Gas Extraction

Onshore Conventional	Offshore Conventional	Associated	Barnett Shale	Marcellus Shale	Coalbed Methane
26.90%	11.30%	13.20%	27.40%	17.10%	4.20%

Conventional onshore natural gas extraction is developed using data from NETL (2010a). Conventional onshore natural gas is recovered by vertical drilling techniques. Once a conventional onshore gas well has been discovered, the natural gas reservoir does not require significant preparation or stimulation for natural gas recovery. Approximately 63 percent of U.S. natural gas production is from conventional onshore gas wells (US EIA, 2009). The conventional onshore gas wells of this analysis are assumed to have a daily production rate between 400 and 1,550 thousand cubic feet, which is characteristic of approximately 40 percent of gas wells in the U.S. (US EIA, 2009b). The key sub-systems for natural gas extraction include compression, dehydration, flaring, water use, and water quality. Table 20 provides the energy and environmental data for the extraction of 1,000 pounds and 1,000 kilograms of natural gas by the conventional onshore method.

Table 20. LCI Data for Natural Gas Extraction (Conventional Onshore)

	1,000 lb		1,000 kg	
Energy				
Process Energy				
Natural gas	913	ft^3	57.0	m^3
Environmental Emissions				
Atmospheric Emissions				
Carbon dioxide	112	lb	112	kg
Methane	1.53	lb	1.53	kg
Nitrous oxide	1.7E-04	lb	1.7E-04	kg
Nitrogen oxides	3.62	lb	3.62	kg
Sulfur dioxide	5.2E-04	lb	5.2E-04	kg
Carbon monoxide	0.28	lb	0.28	kg
NMVOC, non-methane volatile organic compounds,	0.11	lb	0.11	kg
Particulates, > 2.5 um, and < 10um	0.0089	lb	0.0089	kg
Waterborne Releases				
Dissolved solids	3.91	lb	3.91	kg
Boron	0.0019	lb	0.0019	kg
Chloride	0.38	lb	0.38	kg
Sulfate	1.51	lb	1.51	kg
Hydrocarbons, unspecified	0.027	lb	0.027	kg
Solid Wastes				
Solid waste, process to landfill	24.7	lb	24.7	kg
Water Consumption				
Water, surface water consumption	38.2	gal	319	l
Water, groundwater consumption	38.2	gal	319	l

Sources: US EIA 2017e, US EIA 2014, NETL 2010a, US EIA 2009a, US EIA 2009b

Conventional offshore natural gas extraction is developed using data from NETL (2010b). Conventional offshore natural gas is recovered by vertical drilling techniques. Once a conventional offshore gas well has been discovered, the natural gas reservoir does not require significant preparation or stimulation for natural gas recovery. A natural gas reservoir must be large in order to justify the capital outlay for the completion of the well and construction of an offshore drilling platform. The majority of U.S. offshore wells are in the Gulf of Mexico. This analysis assumes that an offshore well produces 25 million cubic feet of natural gas per day (Offshore-technology.com, 2010). Table 21 provides the energy and environmental data for the extraction of 1,000 pounds and 1,000 kilograms of natural gas by the conventional offshore method.

Table 21. LCI Data for Natural Gas Extraction (Conventional Offshore)

	1,000 lb	1,000 kg
Energy		
Process Energy		
Natural gas	844 ft^3	52.7 m^3
Gasoline	0.0041 gal	3.4E-05 m^3
Environmental Emissions		
Atmospheric Emissions		
Carbon dioxide	105 lb	105 kg
Methane	0.43 lb	0.43 kg
Nitrous oxide	0.0026 lb	0.0026 kg
Nitrogen oxides	0.11 lb	0.11 kg
Sulfur dioxide	0.0028 lb	0.0028 kg
Carbon monoxide	0.025 lb	0.025 kg
NMVOC, non-methane volatile organic compounds,	0.0017 lb	0.0017 kg
Particulates, > 2.5 um, and < 10um	0.0054 lb	0.0054 kg
Waterborne Releases		
BOD5, Biological Oxygen Demand	0.99 lb	0.99 kg
TOC, Total Organic Carbon	0.61 lb	0.61 kg
Nitrogen, total	0.044 lb	0.044 kg
Phosphorus, total	5.9E-04 lb	5.9E-04 kg
Dissolved solids	46.7 lb	46.7 kg
Solid Wastes		
Solid waste, process to landfill	24.7 lb	24.7 kg

Sources: US EIA 2017e, US EIA 2014, NETL 2010b, US EIA 2009a, and Offshore-technology.com 2010.

Conventional onshore associated natural gas extraction is developed using data from NETL (2010c). Associated natural gas is co-extracted with crude oil. The extraction of onshore associated gas is similar to the extraction methods for conventional onshore gas. The use of oil/gas separators is necessary to recover natural gas from the mixed product stream. The majority of these wells are assumed to be in Texas and Louisiana (US EIA, 2009c). The production rates of onshore associated gas wells are highly variable, but an average associated gas well in the U.S. produces 59 barrels of oil and 61 thousand cubic feet of natural gas per day (US EIA, 2009b). Table 22 provides the energy and environmental data for the extraction of 1,000 pounds and 1,000 kilograms of associated natural gas by the conventional onshore method.

Table 22. LCI Data for Associated Natural Gas Extraction (Conventional Onshore)

	1,000 lb		1,000 kg	
Energy				
Process Energy				
Natural gas	913	ft^3	57.0	m^3
Environmental Emissions				
Atmospheric Emissions				
Carbon dioxide	112	lb	112	kg
Methane	2.53	lb	2.53	kg
Nitrous oxide	1.7E-04	lb	1.7E-04	kg
Nitrogen oxides	3.62	lb	3.62	kg
Sulfur dioxide	5.2E-04	lb	5.2E-04	kg
Carbon monoxide	0.28	lb	0.28	kg
NMVOC, non-methane volatile organic compounds,	0.21	lb	0.21	kg
Particulates, > 2.5 um, and < 10um	0.0089	lb	0.0089	kg
Waterborne Releases				
Dissolved solids	3.91	lb	3.91	kg
Boron	0.0019	lb	0.0019	kg
Chloride	0.38	lb	0.38	kg
Sulfate	1.51	lb	1.51	kg
Hydrocarbons, unspecified	0.027	lb	0.027	kg
Solid Wastes				
Solid waste, process to landfill	24.7	lb	24.7	kg
Water Consumption				
Water, surface water consumption	38.2	gal	319	l
Water, groundwater consumption	38.2	gal	319	l

Sources: US EIA 2017e, US EIA 2014, NETL 2010c, US EIA 2009a, US EIA 2009b, and US EIA 2009c.

The **Barnett shale gas extraction** is developed using data from NETL (2010d), while the **Marcellus shale gas extraction** is developed using the water use data from NETL (2010e) and the rest of the inputs and outputs from that of the Barnett shale extraction (NETL, 2010d). Natural gas is dispersed throughout the Barnett Shale formation in northern Texas and the Marcellus Shale in the northern Appalachian Basin. Shale gas cannot be recovered using conventional extraction technologies but is recovered through the use of horizontal drilling and hydraulic fracturing (hydrofracking). Horizontal drilling creates a wellbore that runs the length of a shale formation, and hydrofracking uses high pressure fluid (a mixture of water, surfactants, and proppants) for breaking apart the shale reservoir and facilitating the flow of natural gas. Approximately 11 percent of new pipeline capacity in 2008 (4.8 billion cubic feet per day) was installed for natural gas from Barnett Shale (US EIA, 2009c). In 2012, the overall Appalachian natural gas production was 7.8 billion cubic feet per day and has increased to 23.8 billion cubic feet per day in 2017 (US EIA, 2017f). The Marcellus shale unit process is based on the Barnet shale gas extraction unit process with water inputs from the surface and ground sources specific to the Marcellus region. Table 23 provides the energy and environmental data for the extraction of 1,000 pounds and 1,000 kilograms of Barnett shale natural gas. Table 24 provides the energy and environmental data for the extraction of 1,000 pounds and 1,000 kilograms of Marcellus shale natural gas.

The **Coal Bed Methane (CBM) natural gas extraction** is developed using data from NETL (2010f). Natural gas can be recovered from coal seams using horizontal drilling. Coalbed methane (CBM) was first extracted from coal mines as a safety measure to reduce the explosion hazard posed by methane gas in the mines. Deeper coal formations might require hydraulic fracturing to release the natural gas. The development of a well for coal bed methane requires horizontal drilling followed by a depressurization period during which naturally occurring water is discharged from the coal seam. There are viable coal bed methane deposits nationwide, but the majority of CBM production occurs in the Rocky Mountain region (ALL Consulting, 2004). Table 25 provides the energy and environmental data for the extraction of 1,000 pounds and 1,000 kilograms of natural gas from coal bed methane.

Table 23. LCI Data for Barnett Shale Natural Gas Extraction

	1,000 lb		1,000 kg	
Energy				
Process Energy				
Electricity from grid	21.0	kWh	46.2	kWh
Natural gas	698	ft^3	43.6	m^3
Environmental Emissions				
Atmospheric Emissions				
Carbon dioxide	86.3	lb	86.3	kg
Methane	1.27	lb	1.27	kg
Nitrous oxide	1.1E-04	lb	1.1E-04	kg
Nitrogen oxides	2.86	lb	2.86	kg
Sulfur dioxide	4.1E-04	lb	4.1E-04	kg
Carbon monoxide	0.22	lb	0.22	kg
NMVOC, non-methane volatile organic compounds,	0.083	lb	0.083	kg
Particulates, > 2.5 um, and < 10um	0.0070	lb	0.0070	kg
Waterborne Releases				
Dissolved solids	3.72	lb	3.72	kg
Calcium	0.20	lb	0.20	kg
Iron	0.0011	lb	0.0011	kg
Chloride	2.05	lb	2.05	kg
Sulfate	0.0080	lb	0.0080	kg
Magnesium	0.025	lb	0.025	kg
Silicate	7.4E-04	lb	7.4E-04	kg
Solid Wastes				
Solid waste, process to landfill	24.7	lb	24.7	kg
Water Consumption				
Water, surface water consumption	66.0	gal	551	l
Water, groundwater consumption	99.0	gal	826	l

Sources: US EPA 2018, US EIA 2017e, US EIA 2014, NETL 2010d, US EIA 2009a, Hayden 2005, and US EIA 2017f.

Table 24. LCI Data for Marcellus Shale Natural Gas Extraction

	1,000 lb		1,000 kg	
Energy				
Process Energy				
Electricity from grid	21.0	kWh	46.2	kWh
Natural gas	698	ft^3	43.6	m^3
Environmental Emissions				
Atmospheric Emissions				
Carbon dioxide	86.3	lb	86.3	kg
Methane	1.27	lb	1.27	kg
Nitrous oxide	1.1E-04	lb	1.1E-04	kg
Nitrogen oxides	2.86	lb	2.86	kg
Sulfur dioxide	4.1E-04	lb	4.1E-04	kg
Carbon monoxide	0.22	lb	0.22	kg
NMVOC, non-methane volatile organic compounds,	0.083	lb	0.083	kg
Particulates, > 2.5 um, and < 10um	0.0070	lb	0.0070	kg
Waterborne Releases				
Dissolved solids	3.72	lb	3.72	kg
Calcium	0.20	lb	0.20	kg
Iron	0.0011	lb	0.0011	kg
Chloride	2.05	lb	2.05	kg
Sulfate	0.0080	lb	0.0080	kg
Magnesium	0.025	lb	0.025	kg
Silicate	7.4E-04	lb	7.4E-04	kg
Solid Wastes				
Solid waste, process to landfill	24.7	lb	24.7	kg
Water Consumption				
Water, surface water consumption	80.9	gal	675	l
Water, groundwater consumption	1.27	gal	10.6	l

Sources: US EPA 2018, US EIA 2017e, US EIA 2014, NETL 2010d, NETL 2010e, US EIA 2009d, Hayden 2005, and US EIA 2017f.

Table 25. LCI Data for Natural Gas Extraction from Coal Bed Methane

	1,000 lb	1,000 kg
Energy		
Process Energy		
Natural gas	907 ft^3	56.6 m^3
Environmental Emissions		
Atmospheric Emissions		
Carbon dioxide	112 lb	112 kg
Methane	1.56 lb	1.56 kg
Nitrous oxide	1.1E-04 lb	1.1E-04 kg
Nitrogen oxides	3.81 lb	3.81 kg
Sulfur dioxide	5.5E-04 lb	5.5E-04 kg
Carbon monoxide	0.30 lb	0.30 kg
NMVOC, non-methane volatile organic compounds,	0.11 lb	0.11 kg
Particulates, > 2.5 um, and < 10um	0.0093 lb	0.0093 kg
Waterborne Releases		
Dissolved solids	50.8 lb	50.8 kg
Calcium	0.62 lb	0.62 kg
Chloride	12.4 lb	12.4 kg
Sulfate	0.050 lb	0.050 kg
Magnesium	0.20 lb	0.20 kg
Barium	3.56 lb	3.56 kg
Bicarbonate, ion	25.2 lb	25.2 kg
Manganese	0.18 lb	0.18 kg
Sodium	11.9 lb	11.9 kg
Solid Wastes		
Solid waste, process to landfill	24.7 lb	24.7 kg

Sources: US EPA 2018, US EIA 2017e, US EIA 2014, NETL 2010f, US EIA 2009a, and ALL Consulting 2004.

NATURAL GAS PROCESSING

Once raw natural gas is extracted, it is processed to yield a marketable product. First, the heavier hydrocarbons such as ethane, butane and propane are removed and marketed as liquefied petroleum gas (LPG) or feedstocks to chemical processes. Then the water vapor, carbon dioxide, and nitrogen are removed to increase the quality and heating value of the natural gas. If the natural gas has a high hydrogen sulfide content, it is considered “sour.” Before it is used, hydrogen sulfide is removed by adsorption in an amine solution—a process known as “sweetening” (US EIA, 2018).

Natural gas transported on the mainline natural gas transportation system in the United States must meet specific quality measures so that the pipeline network (or grid) can provide uniform quality natural gas. Wellhead natural gas may contain contaminants and hydrocarbon gas liquids (HGL) that must be removed before the natural gas can be safely delivered to the high-pressure, long-distance pipelines that transport natural gas to consumers (US EIA, 2018).

A natural gas processing plant typically receives natural gas from a gathering system of pipelines from natural gas and oil wells. Natural gas processing can be complex and usually involves several processes, or stages, to remove oil, water, HGL, and other impurities such as sulfur, helium, nitrogen, hydrogen sulfide, and carbon dioxide. The composition of the wellhead natural gas determines the number of stages and the processes required to produce pipeline-quality dry natural gas. These stages and processes may be integrated into one unit or operation, be performed in a different order or at alternative locations (lease/plant), or not be required at all (US EIA, 2018).

In the gas processing plant, there are basic stages that the natural gas may go through during processing/treatment. A description of each of these stages are listed here.

- Gas-oil-water separators: Pressure relief in a single-stage separator causes a natural separation of the liquids from the gases in the natural gas. In some cases, a multi-stage separation process is required to separate the different fluid streams.
- Condensate separator: Condensates are most often removed from the natural gas stream at the wellhead with separators much like gas-oil-water separators. The gas flow into the separator comes directly from the wellhead. Extracted condensate is sent to storage tanks.
- Dehydration: A dehydration process removes water that may cause the formation of undesirable hydrates and water condensation in pipelines.
- Contaminant removal: Nonhydrocarbon gases—such as hydrogen sulfide, carbon dioxide, water vapor, helium, nitrogen, and oxygen—must also be removed from the natural gas stream. The most common removal technique is to direct the natural gas though a vessel containing an amine solution. Amines absorb hydrogen sulfide and carbon dioxide from natural gas and can be recycled and regenerated for repeated use. For natural gas that is sweetened, the majority of the H2S removed is used for production of sulfur (USGS, 2008). SO2 is emitted from crude oil and natural gas production and processing operations that handle and treat sulfur-rich, or “sour,” gas. Sulfur dioxide emissions are reported for flaring of H_2S that is not used for recovered sulfur production (Lattanzio, 2018).
- Nitrogen extraction: Once the hydrogen sulfide and carbon dioxide are reduced to acceptable levels, the natural gas stream is routed to a Nitrogen Rejection Unit (NRU), where it is further dehydrated using molecular sieve beds.
- Methane separation: The process of demethanizing the natural gas stream can occur as a separate operation in a natural gas processing plant or as part of the NRU operation. Cryogenic processing and absorption methods are some of the ways used to separate methane from HGL.

- Fractionation: Fractionation separates the HGL into component liquids using the varying boiling points of the individual HGL. HGL from the processing plant may be sent to petrochemical plants, oil refineries, and other HGL consumers (US EIA, 2018).

Once the natural gas has been processed, pipelines move natural gas from the processing plant to markets. Natural gas transmission pipelines are wide-diameter pipelines and are often the long-distance portion of natural gas pipeline systems that connect gathering systems in producing areas, natural gas processing plants, other receipt points, and the main consumer service areas. The three types of transmission pipelines are interstate natural gas pipelines (across state borders), intrastate natural gas pipelines (within a state), and Hinshaw natural gas pipelines (receive from interstate and deliver to consumers). When natural gas arrives at the communities where it will be used (usually through large pipelines), it flows into smaller diameter pipelines called mains and then into smaller service lines that go directly to homes or buildings (US EIA, 2018).

Two natural gas processing unit processes were used in this analysis, one for conventional natural gas and one for shale-derived natural gas. The inputs and emissions data for both these processes are based on the GREET 2017 model (ANL, 2017). For both conventional and shale-derived natural gas processing unit processes, the inputs include energy and water, and outputs include emissions to air. Extracted natural gas is transported primarily by pipeline. Pipeline transportation data were calculated from the total marketed production of natural gas in the U.S. in 2017 (EIA, 2017g) and the annual mileage of natural gas transmission and gathering pipeline in the U.S. (PHMSA, 2018).

Table 26 shows the energy and emissions data for processing 1,000 pounds and 1,000 kilograms of conventional natural gas. Table 27 provides the LCI data from processing 1,000 pounds and 1,000 kilograms of shale-derived natural gas.

Table 26. LCI Data for Conventional Natural Gas Processing

	1,000 lb		1,000 kg	
Material Inputs				
Natural gas	1000	lb	1000	kg
Energy				
Process Energy				
Electricity from grid	4.85	kWh	10.7	kWh
Natural gas	10.9	ft^3	0.68	m^3
Diesel	0.040	gal	3.3E-04	m^3
Transportation Energy				
Pipeline	0.12	ton·mi	0.38	tonne·km
Environmental Emissions				
Atmospheric Emissions				
VOC, volatile organic compounds	0.20	lb	0.20	kg
Carbon monoxide	0.093	lb	0.093	kg
Nitrogen oxides	0.12	lb	0.12	kg
Particulates, < 10 um	0.0054	lb	0.0054	kg
Particulates, < 2.5 um	0.0049	lb	0.0049	kg
Sulfur oxides	0.45	lb	0.45	kg
Methane	0.27	lb	0.27	kg
Nitrogen dioxide	5.1E-04	lb	5.1E-04	kg
Carbon dioxide, fossil	0.095	lb	0.095	kg
Water Consumption	34.5	gal	288	l

Sources: ANL 2017, US EIA 2018, USGS 2008, Lattanzio 2018, US EIA 2017g, PHMSA 2018.

Table 27. LCI Data for Shale-Derived Natural Gas Processing

	1,000 lb		1,000 kg	
Material Inputs				
Natural gas	1000	lb	1000	kg
Energy				
Process Energy				
Electricity from grid	4.85	kWh	10.7	kWh
Natural gas	10.9	ft^3	0.68	m^3
Diesel	0.040	gal	3.3E-04	m^3
Transportation Energy				
Pipeline	0.12	ton·mi	0.38	tonne·km
Environmental Emissions				
Atmospheric Emissions				
VOC, volatile organic compounds	0.20	lb	0.20	kg
Carbon monoxide	0.097	lb	0.097	kg
Nitrogen oxides	0.13	lb	0.13	kg
Particulates, < 10 um	0.0059	lb	0.0059	kg
Particulates, < 2.5 um	0.0054	lb	0.0054	kg
Sulfur oxides	0.45	lb	0.45	kg
Methane	0.27	lb	0.27	kg
Nitrogen dioxide	6.5E-04	lb	6.5E-04	kg
Carbon dioxide, fossil	1.0E-04	lb	1.0E-04	kg
Water Consumption	34.5	gal	288	l

Sources: ANL 2017, US EIA 2018, USGS 2008, Lattanzio 2018, US EIA 2017g, PHMSA 2018.

OLEFINS PRODUCTION (ETHYLENE)

The primary process used for manufacturing olefins is the thermal cracking, or steam cracking, of saturated hydrocarbons such as ethane, propane, naphtha, and other gas oils.

Typical production of ethylene, propylene, and other coproducts begins when hydrocarbons are fed to the cracking furnace. After being pre-heated by a heat exchanger, mixed with steam and then further heated, the hydrocarbon feed is transferred to a reactor. The temperature is again increased to around 800 Celsius, and the cracked gas products are immediately cooled in quench towers using quench oil or quench water. Fuel oil is separated from the main gas stream in a multi-stage centrifugal compressor. The main gas stream then undergoes acid gas removal and drying to remove any moisture that may remain from the quenching process prior to cracked gas compression. The final step involves fractional distillation of the various reaction products and is achieved using a series of distillation columns and hydrogenation reactors.

Within the hydrocracker, an offgas is produced from the raw materials entering. A portion of this offgas is processed and used as fuel gas to produce steam for the hydrocracker, while the remaining portion is exported from the hydrocracker as a coproduct. This internally created energy is included in the analysis by including the production of the raw materials combusted to produce the energy as well as the energy amount attributed to the combustion of those raw materials. Unlike the raw materials that become part of the product output mass, no material feedstock energy is assigned to the raw materials inputs that are combusted within the process. This offgas used within the process is shown as a weight of natural gas and petroleum input to produce the energy, as well as the energy amount produced from those weights.

An individual weighted average for three leading ethylene producers (10 thermal cracking units) was calculated using ethylene production amounts from each plant. All companies provided data for the year 2015. A weighted average was calculated from the data collected and used to develop the LCA model. Propylene, pyrolysis gasoline and butadiene are among the coproducts of ethylene production, and a mass basis was used to allocate the credit for the coproducts. Numerous coproduct streams are produced during this process. Fuel gas and off-gas were two of the coproducts produced that were exported to another process for fuel use. For coproducts sold for fuel use in other processes, these were treated as an avoided fuel product and were given credits based on the fuel they would replace.

The captured ethylene production amount is approximately 10 percent of the ethylene production in the U.S. in 2015 (OGJ, 2017). While data was collected from a relatively small sample of plants, the olefins producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American olefins production. All data collected and the average olefins LCI data were individually reviewed by the data providers.

To assess the quality of the data collected for olefins, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for olefins include direct measurements, information provided by purchasing and utility records, and estimates. The standard production technology for olefins is the steam cracking of hydrocarbons (including natural gas liquids and petroleum liquids). The data in this module represent steam cracking of natural gas and petroleum products. All data submitted for olefins represent the year 2015 and U.S. and Canada production.

Table 28 shows the averaged energy and emissions data for the production of 1,000 pounds and 1,000 kilograms of ethylene. In the case of some emissions, data was provided by fewer than the 3 producers. To indicate known emissions while protecting the confidentiality of individual company responses, some emissions are reported only by the order of magnitude of the average.

Table 28. LCI Data for the Production of Ethylene

	1,000 lb		1,000 kg		
Material Inputs (1)					
Refined Petroleum Products	104	lb	104	kg	
Processesed Natural Gas	896	lb	896	kg	
Internal off-gas (2)					
From oil	19.4	lb	19.4	kg	
From natural gas	154	lb	154	kg	
Energy					
Process Energy					
Electricity from grid	12.7	kWh	28.0	kWh	
Electricity from cogen	12.2	kWh	27.0	kWh	
Natural gas	1,787	ft^3	112	m^3	
Fuel Gas	1,424	ft^3	88.9	m^3	
Landfill gas	11.6	ft^3	0.72	m^3	
Avoided Energy					
Oil sold as co-product	0.37	gal	0.0031	m^3	
Recovered energy from exported steam	217	ft^3	13.6	m^3	
Off-gas sold	794	ft^3	49.5	m^3	
Transportation Energy					
Barge	25.8	ton·mi	83.0	tonne·km	
Pipeline -refinery products	0.48	ton·mi	1.56	tonne·km	
Pipeline -natural gas products	256	ton·mi	826	tonne·km	
Environmental Emissions					
Atmospheric Emissions					
Particulates, unspecified	0.010	lb	0.010	kg	*
Particulates, < 2.5 um	0.025	lb	0.025	kg	
Particulates, > 2.5 um, and < 10um	0.0049	lb	0.0049	kg	
Nitrogen oxides	0.29	lb	0.29	kg	
NMVOC, non-methane volatile organic compounds,	0.12	lb	0.12	kg	
VOC, volatile organic compounds	0.010	lb	0.010	kg	*
Sulfur oxides	0.020	lb	0.020	kg	
Carbon dioxide, fossil	640	lb	640	kg	
Methane, fossil	0.10	lb	0.10	kg	
Nitrous oxide	0.20	lb	0.20	kg	
Carbon monoxide	0.26	lb	0.26	kg	
Hydrogen sulfide	1.0E-06	lb	1.0E-06	kg	*
Ammonia	0.0010	lb	0.0010	kg	*
Chlorine	1.0E-05	lb	1.0E-05	kg	*

Table 28. LCI Data for the Production of Ethylene (Continued)

	1,000 lb	1,000 kg	
Environmental Emissions			
Waterborne Releases			
Benzene	0.010 lb	0.010 kg	*
BOD5, Biological Oxygen Demand	0.0039 lb	0.0039 kg	
COD, Chemical Oxygen Demand	0.40 lb	0.40 kg	
Benzene, ethyl-	0.0010 lb	0.0010 kg	*
Phenol	1.0E-04 lb	1.0E-04 kg	*
Styrene	0.010 lb	0.010 kg	*
Suspended solids, unspecified	0.010 lb	0.010 kg	*
Toluene	0.010 lb	0.010 kg	*
TOC, Total Organic Carbon	1.0E-06 lb	1.0E-06 kg	*
Xylene	0.0010 lb	0.0010 kg	*
Dissolved solids	1.0E-05 lb	1.0E-05 kg	*
Cyanide	1.0E-06 lb	1.0E-06 kg	*
Nickel	1.0E-06 lb	1.0E-06 kg	*
Mercury	1.0E-07 lb	1.0E-07 kg	*
Lead	1.0E-07 lb	1.0E-07 kg	*
Ammonia	0.0010 lb	0.0010 kg	*
Ethylene glycol	0.0010 lb	0.0010 kg	*
Propylene glycol	0.0010 lb	0.0010 kg	*
Ethene	0.010 lb	0.010 kg	*
Butadiene	0.0010 lb	0.0010 kg	*
Isoprene	1.0E-04 lb	1.0E-04 kg	*
Cresol	1.0E-05 lb	1.0E-05 kg	*
Biphenyl	0.0010 lb	0.0010 kg	*
7,12-Dimethylbenz(a)anthracene	1.0E-05 lb	1.0E-05 kg	*
3-Methylcholanthrene	1.0E-06 lb	1.0E-06 kg	*
Sodium Bisulfate	1.0E-05 lb	1.0E-05 kg	*
Dimethyl phthalate	1.0E-04 lb	1.0E-04 kg	*
Dibenz(a,j)acridine	1.0E-06 lb	1.0E-06 kg	*
Solid Wastes			
Solid waste, process to landfill	0.32 lb	0.32 kg	
Solid waste, process to incineration	6.00 lb	6.00 kg	
Solid waste, process to waste-to-energy incineratior	6.1E-04 lb	6.1E-04 kg	
Solid Waste Sold for Recycling or Reuse	0.30 lb	0.30 kg	
Hazardous waste to landfill	0.0031 lb	0.0031 kg	
Hazardous waste to incineration	1.40 lb	1.40 kg	

Table 28. LCI Data for the Production of Ethylene (Continued)

	1,000 lb		1,000 kg	
Water Consumption	419	gal	3,500	l

* To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by the order of magnitude of the average.

(1) Specific input materials from oil refining and natural gas processing include ethane, propane, liquid feed, heavy raffinate, and DNG.

(2) A portion of the material feed combusts within the hydrocracker and produces an offgas, which provides an internal energy source

Source: Primary Data, 2018(a)

OXYGEN PRODUCTION

Oxygen is manufactured by cryogenic separation of air. This technique is essentially one of liquefying air, then collecting the oxygen by fractionation. The oxygen is produced in the form of a liquid, which boils at 184° Celsius below zero at normal atmospheric pressure, so it must be kept under stringent conditions of temperature and pressure for handling. Most oxygen plants are located quite close to their point of consumption and use pipelines to minimize transportation difficulties, although there is a small amount of long-distance hauling in insulated rail cars.

The energy data for producing 1,000 pounds and 1,000 kilograms oxygen is displayed in Table 29. The data used has been adapted from EcoInvent 2.2. Electricity is linked to the US electricity grid. Infrastructure has been removed from the process. Rail transport was also removed as it was uncertain whether the mode and mileage were representative of the US.

Table 29. Data for the Production of Oxygen

	1,000 lb		1,000 kg	
Inputs from Nature				
Oxygen (in air)	1000	lb	1000	kg
Water (cooling, consumed)	311	gal	2.59	m^3
Energy				
Process Energy				
Electricity from grid	349	kWh	769	kWh
Environmental Emissions				
Atmospheric Emissions				
Heat, waste	2.62	MM Btu	2,768	MJ

Source: Althaus, 2007

ETHYLENE OXIDE/ETHYLENE GLYCOL PRODUCTION

Ethylene Oxide Production

The primary production method for ethylene oxide is the direct, vapor-phase oxidation of ethylene with air or oxygen over a catalyst at a high temperature and pressure (DOW, 2009). The predominant feed for commercial oxidation processes is oxygen rather than air due to higher yields and less downtime (GCI, 2010). While most manufacturers of ethylene oxide purchase the oxygen needed in the reaction, some plants pull oxygen from air separation on-site. The ethylene oxide is catalyzed by silver and is exothermic. Oil or boiling water is used to absorb the heat in a multi-tubular catalytic reactor and produce steam that is used in other parts of the process. The products of the reaction are fed to an ethylene oxide absorber for lights removal by water quenching. Part of the gaseous stream is recycled into the multi-tubular reactor, while the other part is sent to a CO2 removal unit consisting of an absorber and a stripper (Chem, 2015). Because of its special molecular structure, ethylene oxide easily participates in the addition reaction and can easily polymerize into larger compounds (GCI, 2010).

A disadvantage to the oxidation process is the conversion of ethylene to carbon dioxide at a ratio of 6:2 (GCI, 2010) and water, which is released to the environment. However, excess ethylene is added to prevent additional oxidation of the ethylene oxide that would increase the production of carbon dioxide. This creates typical conversion rates for ethylene to ethylene oxide of only 10 to 20 percent per pass. Approximately 20 to 25 percent of the ethylene is broken down to carbon dioxide and water. Additionally, gases from the catalytic reaction are cooled and then passed through a scrubber where the ethylene oxide is absorbed as a dilute aqueous solution. This process includes the removal of CO2 using physical sorbents, the Hot Potassium Carbonate process, or cryogenic separation techniques (GCI, 2010)

The energy requirements and environmental emissions for the production of ethylene oxide are shown as an aggregate with ethylene glycol in Table 30. These data include a weighted average of 3 ethylene oxide producers with 5 plants in the U.S. from 2015-2016.

Ethylene Glycol Production

Ethylene glycol is primarily produced by the hydration of ethylene oxide, but it can also be produced via acetoxylation and coal gasification processes (Huntsman, 2000). Only the hydration of ethylene oxide is included in this dataset. The production process is generally close to the process unit for ethylene oxide. The ethylene glycol production reaction can occur uncatalyzed, or catalyzed with an acid or a base, or at neutral pH under high temperatures. An uncatalyzed reaction is much slower, but acid removal from the glycol is required if an acidic catalyst is used.

While basic catalysts significantly increase the production of higher glycols (Choudhari, 2001) he biggest yields of ethylene glycol – around 90% - are produced at an acidic or neutral pH with a large excess of water added to the reactor feed (MEGlobal, 2013). Almost all the ethylene oxide is reacted. A mixture of cold recycle water, ethylene oxide, and pure water is first created. The solution is pumped through preheaters into an adiabatic reactor where the ethylene oxide is hydrated, and a glycol mixture is produced (Choudhari, 2001). This glycol/water mixture is sent through an evaporator to concentrate the solution and recover evaporated water. Meanwhile, condensate is recycled back to the feed tank to be used to prepare the ethylene oxide feed. High purity ethylene glycol is obtained from the concentrated glycol solution by vacuum distillation.

The excess water used to increase product yields does so through reducing the amount of byproduct produced. After the water-glycol mixture is fed to evaporators, this excess water is recovered and recycled. The major byproducts of the reaction are ethylene glycol oligomers, diethylene glycol, triethylene glycol, and tetraethylene glycol (MEGlobal, 2013). The ethylene glycol is separated from these by-products through a process of fractional distillation under a vacuum (ICIS, 2010). Mono- and di-ethylene glycol (MEG and DEG) are both represented in the data collected.

Bio-based ethylene glycol is being used for less than 5 percent of the total average EG input and is used by a limited number of PET producers. At this time, the amount of bio-based EG provided by PET manufacturers has been included as petroleum based EG. The amount of bio-based EG will be reassessed at the next update to determine if it is necessary to include as a material input.

Data was collected from three leading ethylene oxide/ethylene glycol producers (7 EO/EG plants). When ethylene oxide and ethylene glycol data were provided separately for a company, an aggregated ethylene oxide/ethylene glycol data set was prepared for that company. For producers that provided data from more than one plant, a weighted average using production amounts from each plant for the individual company was created. The average for each producer was then used to determine the overall weighted average for ethylene oxide/ethylene glycol production in North America. The average data set was individually reviewed by the data providers.

To assess the quality of the data collected for ethylene oxide/ethylene glycol, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for ethylene oxide/ethylene glycol include direct measurements, information provided by purchasing and utility records, and estimates. The standard production technology for ethylene oxide is the direct, vapor-phase oxidation of ethylene with air or oxygen over a catalyst. The production technology for ethylene glycol is the hydration of ethylene oxide. All data submitted for ethylene oxide and ethylene glycol represent the years 2015 and 2016 and U.S. production.

Table 30 shows the averaged energy and emissions data for the production of 1,000 pounds and 1,000 kilograms of ethylene glycol, including ethylene oxide production. To indicate known emissions while protecting the confidentiality of individual company responses, some emissions are reported only by the order of magnitude of the average.

Table 30. Data for the Production of Ethylene Glycol (Including Ethylene Oxide)

	1,000 lb		1,000 kg		
Material Inputs					
Ethylene	588	lb	588	kg	
Oxygen	565	lb	565	kg	
Water	238	gal	0.24	m^3	
Nitrogen	10.2	lb	10.2	kg	
Energy					
Process Energy					
Electricity from grid	67	kWh	148	kWh	
Electricity from cogen	40	kWh	88	kWh	
Natural gas	2331	ft^3	146	m^3	
Avoided Energy					
Recovered energy from steam	349	ft^3	22	m^3	
Transportation Energy					
Pipeline	10.6	ton·mi	34.0	tonne·km	
Environmental Emissions					
Atmospheric Emissions					
Particulates	0.0010	lb	0.0010	kg	*
Particulates, < 2.5 um	1.0E-05	lb	1.0E-05	kg	*
Particulates, > 2.5 um, and < 10um	1.0E-04	lb	1.0E-04	kg	*
Nitrogen oxides	0.010	lb	0.010	kg	*
NMVOC, non-methane volatile organic compounds,	0.010	lb	0.010	kg	*
Hydrocarbons, unspecified	0.010	lb	0.010	kg	*
Sulfur oxides	1.0E-07	lb	1.0E-07	kg	*
Carbon dioxide, fossil	320	lb	320	kg	
Methane	0.010	lb	0.010	kg	*
Nitrous oxide	0.0010	lb	0.0010	kg	*
Carbon monoxide	0.0010	lb	0.0010	kg	*
Aldehydes, unspecified	0.0010	lb	0.0010	kg	*
Methanol	1.0E-05	lb	1.0E-05	kg	*
Diethyl ether	1.0E-06	lb	1.0E-06	kg	*
Naphthalene, 1,2,3,4-tetrahydro-	0.0010	lb	0.0010	kg	*
Ethylene Dichloride	1.0E-05	lb	1.0E-05	kg	*
Naphtalene	1.0E-04	lb	1.0E-04	kg	*
Ethylene oxide	0.0010	lb	0.0010	kg	*
Ethylene glycol	1.0E-04	lb	1.0E-04	kg	*
1,4-Dioxane	0.0010	lb	0.0010	kg	*
Ethene	0.0010	lb	0.0010	kg	*
Ethane	1.0E-04	lb	1.0E-04	kg	*

Table 30. Data for the Production of Ethylene Glycol (Including Ethylene Oxide) (Continued)

	1,000 lb		1,000 kg		
Environmental Emissions					
Waterborne Releases					
TOC, Total Organic Carbon	0.10	lb	0.10	kg	*
Ethylene oxide	0.010	lb	0.010	kg	*
Ethylene glycol	1.00	lb	1.00	kg	*
Ethane, 1,2-dichloro-	0.0010	lb	0.0010	kg	*
1,4-Dioxane	0.0010	lb	0.0010	kg	*
Solid Wastes					
Solid waste, process to landfill	1.00	lb	1.00	kg	
Solid waste, process to incineration	0.67	lb	0.67	kg	
Hazardous waste to incineration	0.0054	lb	0.0054	kg	
Hazardous waste to WTE	0.0024	lb	0.0024	kg	
Water Consumption	37.2	gal	310	l	

* To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by the order of magnitude of the average.

Source: Primary Data, 2018(b)

METHANOL PRODUCTION

Methanol is produced through synthesis of a gaseous mixture of hydrogen, carbon monoxide, and carbon dioxide (called syngas). Methanol can be produced from biomass, coal, heavy oil, naphtha, and other feedstocks. Steam-methane reforming (SMR) technology is widely used in existing methanol plants (Wang & Huang, 1999).

According to Wang & Huang (1999), the majority of the total natural gas input in methanol plants is used as feed for syngas production; the remainder is used as process fuel. For SMR plants, 78-88% of the total natural gas input in methanol plants is used as feed. The split of natural gas between feed and fuel is used in GREET model to calculate emissions of criteria pollutants during methanol production. In particular, the amount of natural gas burned and the emission factors of natural gas combustion are used to determine combustion emissions of natural gas used as fuel in methanol plants. Because syngas is pressurized in reformers, fugitive emissions of carbon monoxide and carbon dioxide may be released from reformers. But no data are available to estimate this amount. Emissions are estimated from methanol plants using the Fischer-Tropsch Diesel (FTD) production process. According to Syntroleum researchers, VOC emissions from FTD plants should be equal to those from petroleum refineries (on the basis of per-unit-of-product output); carbon monoxide emissions from FTD plants should be fewer than 100 tons per year for a 1,000-barrel-per-day plant; and NOx emissions should be less than 60 tons per year. Using these values and based on an assumed plant capacity of 85%, a carbon monoxide emission rate is estimated to be 58.6 g/million Btu of fuel output and nitrogen oxides emission rate of 35.2 g/million Btu. These emissions rates are based on manufacturer-suggested emissions limits. In the GREET simulation, only half of these estimated emissions rates are assumed (Wang & Huang, 1999).

The inputs and emissions data for methanol are taken from GREET 2017 and the data for hazardous and non-hazardous waste material is taken from an industrial leader in methanol production. The transportation energy was estimated from discussions with an acetic acid producer.

Table 31 shows the energy and emissions data for the production of 1,000 pounds and 1,000 kilograms of methanol.

CARBON MONOXIDE PRODUCTION

Carbon monoxide is produced as a co-product of conventional hydrogen production process of steam-methane reformation. Steam-methane reforming (SMR) is a mature production process in which high-temperature steam (700°C–1,000°C) is used to produce hydrogen from a methane source, such as natural gas. In steam-methane reforming, methane reacts with steam under 3–25 bar pressure (1 bar = 14.5 psi) in the presence of a catalyst to produce hydrogen, carbon monoxide, and a relatively small amount of carbon dioxide. Steam reforming is endothermic—that is, heat must be supplied to the process for the reaction to proceed (Susmozas, 2013).

Subsequently, in what is called the "water-gas shift reaction," the carbon monoxide and steam are reacted using a catalyst to produce carbon dioxide and more hydrogen. In a final process step called "pressure-swing adsorption," carbon dioxide and other impurities are removed from the gas stream, leaving essentially pure hydrogen. Steam reforming can also be used to produce hydrogen from other fuels, such as ethanol, propane, or even gasoline.

Table 32 shows the averaged energy and emissions data for the production of 1,000 pounds and 1,000 kilograms of carbon monoxide.

Table 31. Data for the Production of Methanol

	1,000 lb		1,000 kg	
Material Inputs				
Oxygen	380	lb	380	kg
Natural gas	620	lb	620	kg
Energy				
Process Energy				
Electricity from grid	114	kWh	252	kWh
Natural gas	118	ft^3	7.37	m^3
Transportation Energy				
Pipeline	155	ton·mi	499	tonne·km
Environmental Emissions				
Atmospheric Emissions				
Carbon dioxide, fossil	390	lb	390	kg
VOC, volatile organic compounds	0.50	lb	0.50	kg
Carbon monoxide	0.72	lb	0.72	kg
Nitrogen oxides	1.11	lb	1.11	kg
Particulates, < 10 um	0.26	lb	0.26	kg
Particulates, < 2.5 um	0.26	lb	0.26	kg
Sulfur oxides	0.33	lb	0.33	kg
Methane	4.59	lb	4.59	kg
Nitrogen dioxide	0.010	lb	0.010	kg
Solid Wastes				
Non-hazardous waste to landfill	0.26	lb	0.26	kg
Solid Waste Sold for Recycling or Reuse	0.21	lb	0.21	kg
Hazardous waste for disposal	0.0069	lb	0.0069	kg
Hazardous waste, recovery	0.0085	lb	0.0085	kg
Water Consumption	47.2	gal	394	l

Sources: Methanex 2016, Franklin 2010b, and ANL 2017.

Table 32. Data for the Production of Carbon Monoxide

	1,000 lb		1,000 kg	
Material Inputs				
Natural gas	684	lb	684	kg
Energy				
Process Energy				
Electricity from grid	33.7	kWh	74.3	kWh
Natural gas	5,289	ft^3	330	m^3
Transportation Energy				
Pipeline	171	ton·mi	250	tonne·km
Environmental Emissions				
Atmospheric Emissions				
Carbon monoxide	6.9	lb	6.9	kg
Organic substances, unspecified	3.6	lb	3.6	kg
Sulfur oxides	0.029	lb	0.029	kg
Water Consumption	67.7	gal	565	liters

Source: NREL 2001, Franklin Associates 2010(a), Franklin Associates 2010(b), US EPA 1995.

MIXED XYLENES PRODUCTION

Mixed xylenes are created as a coproduct of benzene and toluene from one of three sources—pyrolysis gasoline from steam cracking, naphtha from the refining process, or coke oven gas from coal pyrolysis. This analysis considers the production from the catalytic reforming of naphtha from a refinery.

The reforming processes are used to convert paraffinic hydrocarbon streams into aromatic compounds such as benzene, toluene, and xylene. Catalytic reforming uses catalysts, such as platinum and palladium, to dehydrogenate straight-run light naphtha to yield a mixture of aromatic hydrocarbons (Cheremisinoff, 2009). The hydrogen that is removed during dehydrogenation is used during the hydrocracking process and reduces coke formation.

The BTX aromatics are then extracted from the reformate and fractionated to separate streams using distillation. Adsorption or crystallization may be used as well to separate the aromatic streams.

Table 33 displays the energy and emissions data for the production of 1,000 pounds and 1,000 kilograms of mixed xylenes. Total energy data for mixed xylenes were provided by a confidential source in the previous analysis from 2011. The mix of fuels for energy and estimated transport data was reviewed and revised from discussions with a current producer in 2018. Carbon dioxide emissions were estimated from the PlasticsEurope BTX EcoProfile report (PlasticsEurope, 2013).

Table 33. Data for the Production of Mixed Xylenes

	1,000 lb		1,000 kg	
Material Inputs				
Naphtha	1000	lb	1000	kg
Energy				
Process Energy				
Electricity from grid	9.53	kWh	21.0	kWh
Natural gas	817	ft^3	51.0	m^3
Transportation Energy				
Barge	25.9	ton·mi	83.2	tonne·km
Pipeline	5.00	ton·mi	16.1	tonne·km
Environmental Emissions				
Atmospheric Emissions				
Carbon dioxide	150	lb	150	kg

Sources: Primary data 2006, Primary data 2018c, PlasticsEurope 2013

PARAXYLENE PRODUCTION

Reformate feedstock rich in xylenes is fractionated to obtain a stream rich in the para-isomer. The ortho isomer is first separated off by distillation. A crystallization unit is then used to separate the meta and para isomers using adsorption of the paraxylene isomer on a molecular sieve adsorbent. The paraxylene isomer is collected on the adsorbent while the metaxylene passes through the adsorbent bed and is collected. The paraxylene is then stripped of the adsorbent using diethylbenzene isomers. The meta and para isomers can also be separated using crystallization and then centrifuged for purification (Gary, 2007).

LCI data for the production of Paraxylene (PX) was collected from three producers (3 plants) in North America – all in the United States. Not all plants were able to provide data for 2015. One plant provided 2013 data and one provided 2016 data. These variances were due to plant issues (e.g. shut downs/updates/temporary maintenance shut downs) during 2015 that may have skewed the average. Coproducts include a number of aromatics, carbon dioxide, and some fuels. For the coproducts sold for material use in other processes, mass basis was used to allocate the credit for the coproduct. For coproducts sold for fuel use in other processes, these were treated as an avoided fuel product and were given credits based on the fuel they would replace. The average paraxylene datasets were reviewed and accepted respectively by each paraxylene data provider.

To assess the quality of the data collected for TPA/PTA, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for TPA/PTA include direct measurements, information provided by purchasing and utility records, and estimates.

Table 34 shows the averaged energy and emissions data for the production of 1,000 pounds and 1,000 kilograms of paraxylene. To indicate known emissions while protecting the confidentiality of individual company responses, some emissions are reported only by the order of magnitude of the average.

Table 34. Data for the Production of Paraxylene

	1,000 lb		1,000 kg		
Material Inputs					
Mixed Xylenes	996	lb	996	kg	
Nitrogen	4.30	lb	4.30	kg	
Internal off-gas (1)					
From Oil	16.0	lb	16.0	kg	
Energy					
Process Energy					
Electricity from grid	58.8	kWh	130	kWh	
Electricity from cogen	48.4	kWh	107	kWh	
Natural gas	1,006	ft^3	62.8	m^3	
Fuel gas (2)	65.8	ft^3	4.11	m^3	
Avoided Energy					
Fuel gas created from the process and exported	142	ft^3	8.89	m^3	
Transportation Energy					
Barge	216	ton·mi	696	tonne·km	
Ship	31.7	ton·mi	102	tonne·km	
Pipeline	23.9	ton·mi	77.0	tonne·km	
Truck	0.024	ton·mi	0.077	tonne·km	
Environmental Emissions					
Atmospheric Emissions					
Particulates	0.010	lb	0.010	kg	*
Nitrogen oxides	0.010	lb	0.010	kg	*
Sulfur oxides	1.0E-04	lb	1.0E-04	kg	*
Carbon dioxide, in air	0.10	lb	0.10	kg	*
Carbon dioxide, fossil	100	lb	100	kg	*
Methane	1.00	lb	1.00	kg	*
Carbon monoxide	0.010	lb	0.010	kg	*
Hexane	1.0E-04	lb	1.0E-04	kg	*
Ethene	0.0010	lb	0.0010	kg	*
Propene	1.0E-04	lb	1.0E-04	kg	*
Propane	0.010	lb	0.010	kg	*
Butene	1.0E-04	lb	1.0E-04	kg	*
Butane	0.0010	lb	0.0010	kg	*
Benzene	0.0010	lb	0.0010	kg	*
Toluene	1.0E-04	lb	1.0E-04	kg	*
Xylene	0.010	lb	0.010	kg	*
Benzene, ethyl-	0.0010	lb	0.0010	kg	*
Ethane	0.0010	lb	0.0010	kg	*

Table 34. Data for the Production of Paraxylene
(Continued)

	1,000 lb	1,000 kg	
Atmospheric Emissions			
Pentane	1.0E-04 lb	1.0E-04 kg	*
Heptane	1.0E-05 lb	1.0E-05 kg	*
Formaldehyde	1.0E-05 lb	1.0E-05 kg	*
N-octane	1.0E-05 lb	1.0E-05 kg	*
Nonane	1.0E-05 lb	1.0E-05 kg	*
Trimethylbenzenes	1.0E-05 lb	1.0E-05 kg	*
Cumene	1.0E-05 lb	1.0E-05 kg	*
1,3 Butadiene	1.0E-04 lb	1.0E-04 kg	*
1,4-Diethylbenzene	1.0E-05 lb	1.0E-05 kg	*
Methane, bromo-, Halon 1001	1.0E-05 lb	1.0E-05 kg	*
Methanol	0.10 lb	0.10 kg	*
Waterborne Releases			
BOD5, Biological Oxygen Demand	0.0010 lb	0.0010 kg	*
COD, Chemical Oxygen Demand	0.010 lb	0.010 kg	*
Sulfide	1.0E-04 lb	1.0E-04 kg	*
Oils, unspecified	0.0010 lb	0.0010 kg	*
Suspended solids, unspecified	0.0010 lb	0.0010 kg	*
Chromium	1.0E-08 lb	1.0E-08 kg	*
Iron	1.0E-07 lb	1.0E-07 kg	*
Aluminium	1.0E-06 lb	1.0E-06 kg	*
Nickel	1.0E-07 lb	1.0E-07 kg	*
Mercury	1.0E-08 lb	1.0E-08 kg	*
Zinc	1.0E-07 lb	1.0E-07 kg	*
Ammonia	1.0E-06 lb	1.0E-06 kg	*
Cobalt	1.0E-05 lb	1.0E-05 kg	*
Manganese	1.0E-05 lb	1.0E-05 kg	*
Solid Wastes			
Solid waste, process to landfill	0.10 lb	0.10 kg	
Solid Waste Sold for Recycling or Reuse	0.010 lb	0.010 kg	
Hazardous waste to incineration	0.0010 lb	0.0010 kg	
Water Consumption	4.87 gal	40.6 l	

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* To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by the order of magnitude of the average.

(1) A portion of the material feed produces an off-gas which provides an energy source.

(2) imported from external unit at site

Source: Primary Data, 2018(d)

CRUDE TEREPHTHALIC ACID (TPA)/PURIFIED TEREPHTHALIC ACID (PTA) PRODUCTION

The main production method for PTA in North America is by the Amoco technology. Crude terephthalic acid is manufactured primarily by the oxidation of paraxylene in the liquid phase. Liquid paraxylene, acetic acid, and a catalyst, such as manganese or cobalt bromides, are combined as the liquid feed to the oxidizers. The temperature of this exothermic reaction is maintained at about 200° C (Lloyd, 2011). The pressure may range from 300 to 400 psi.

Reactor effluents are continuously removed from the reactor and routed to a series of crystallizers, where they are cooled by flashing the liquids. The partially oxidized impurities are more soluble in acetic acid and tend to remain in solution, while crude TPA crystallizes from the liquor.

The slurry from the crystallizers is sent to solid/liquid separators, where crude TPA is recovered in the solids. The liquid portion is distilled and acetic acid, methyl acetate, and water are recovered overhead. Acetic acid is removed from the solution and recycled back to the oxidizer.

The purification of crude TPA involves the hydrogenation of the crude TPA over a palladium-containing catalyst at about 450°F. High-purity TPA is recrystallized from a high-pressure water solution of the hydrogenated material.

LCI data for the production of TPA/PTA was collected from three producers (three plants) in North America – all in the United States. Not all plants were able to provide data for 2015. One plant provided 2013 data and one provided 2016 data. These variances were due to plant issues (e.g. shut downs/updates/temporary maintenance shut downs) during 2015 that may have skewed the average. Small amounts (less than 1 percent of total output) of off-spec PTA are produced as coproducts during this process. A mass basis was used to allocate the credit for the coproduct. The average TPA/PTA datasets were reviewed and accepted respectively by each TPA/PTA data provider. This dataset also includes the production of acetic acid for use in the process. This is due to confidentiality issues as only one plant provided data for acetic acid from 2006. No new data was collected for acetic acid.

To assess the quality of the data collected for TPA/PTA, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for TPA/PTA include direct measurements, information provided by purchasing and utility records, and estimates.

Table 35 shows the averaged energy and emissions data for the production of 1,000 pounds and 1,000 kilograms of PTA, including TPA production. To indicate known emissions while protecting the confidentiality of individual company responses, some emissions are reported only by the order of magnitude of the average.

Table 35. Data for the Production of TPA/PTA (Including Acetic Acid Production)

	1,000 lb		1,000 kg		
Material Inputs					
Paraxylene	653	lb	653	kg	
Methanol	16.3	lb	16	kg	
Carbon Monoxide	15.1	lb	15	kg	
Oxygen (from air)	757	lb	757	kg	
Energy					
Process Energy					
Electricity from grid	183	kWh	404	kWh	
Electricity from cogen	0.056	kWh	0.12	kWh	
Natural gas	859	ft^3	53.6	m^3	
Avoided Energy					
Off-gas sold as credit	4.70	cuft	0.29	m^3	
Transportation Energy					
Barge	0.41	ton·mi	1.31	tonne·km	
Ship	516	ton·mi	1,659	tonne·km	
Pipeline	0.046	ton·mi	0.15	tonne·km	
Rail	32.2	ton·mi	104	tonne·km	
Truck	8.7E-04	ton·mi	0.0028	tonne·km	
Environmental Emissions					
Atmospheric Emissions					
Acetic acid	0.010	lb	0.010	kg	*
Methyl acetate	0.10	lb	0.10	kg	*
Xylene	0.0010	lb	0.0010	kg	*
Carbon dioxide	43.4	lb	43.4	kg	
Methane	3.32	lb	3.32	kg	
Carbon monoxide	0.15	lb	0.15	kg	
Aldehydes, unspecified	0.0010	lb	0.0010	kg	*
Methane, bromo-, Halon 1001	0.0010	lb	0.0010	kg	*
Methanol	0.034	lb	0.034	kg	
Acetaldehyde	1.0E-04	lb	1.0E-04	kg	*
Methyl formate	1.0E-04	lb	1.0E-04	kg	*
Benzene	0.0010	lb	0.0010	kg	*
Toluene	0.0010	lb	0.0010	kg	*
Formaldehyde	1.0E-04	lb	1.0E-04	kg	*
Benzoic acid	0.0010	lb	0.0010	kg	*
Hydrogen	0.010	lb	0.010	kg	*
Particulates	0.010	lb	0.010	kg	*
Particulates, < 10 um	0.10	lb	0.10	kg	*
Particulates, < 2.5 um	0.010	lb	0.010	kg	*

Table 35. Data for the Production of TPA/PTA (Including Acetic Acid Production) (Continued)

	1,000 lb		1,000 kg		
Environmental Emissions					
Atmospheric Emissions					
Nitrogen oxides	0.010	lb	0.010	kg	*
NMVOC, non-methane volatile organic compounds,	0.10	lb	0.10	kg	*
Sulfur oxides	1.0E-04	lb	1.0E-04	kg	*
Waterborne Releases					
Suspended solids, unspecified	0.010	lb	0.010	kg	*
Sulfide	1.0E-08	lb	1.0E-08	kg	*
BOD5, Biological Oxygen Demand	0.0010	lb	0.0010	kg	*
COD, Chemical Oxygen Demand	0.10	lb	0.10	kg	*
Ammonia	0.0043	lb	0.0043	kg	
TOC, Total Organic Carbon	0.01	lb	0.01	kg	*
Oils, unspecified	0.010	lb	0.010	kg	*
Acetic acid	0.010	lb	0.010	kg	*
Chromium	1.0E-12	lb	1.0E-12	kg	*
Iron	0.010	lb	0.010	kg	*
Aluminum, ion	0.0010	lb	0.0010	kg	*
Nickel	1.0E-05	lb	1.0E-05	kg	*
Mercury	1.0E-12	lb	1.0E-12	kg	*
Lead	1.0E-06	lb	1.0E-06	kg	*
Phosphate	0.0010	lb	0.0010	kg	*
Zinc	1.0E-11	lb	1.0E-11	kg	*
Sulfate	0.10	lb	0.10	kg	*
Magnesium	0.10	lb	0.10	kg	*
Bromide	0.10	lb	0.10	kg	*
Cobalt	0.0010	lb	0.0010	kg	*
Manganese	0.010	lb	0.010	kg	*
Potassium	0.0010	lb	0.0010	kg	*
Benzene	0.0010	lb	0.0010	kg	*
Methanol	0.010	lb	0.010	kg	*
Nitrate	0.010	lb	0.010	kg	*
Solid Wastes					
Solid waste process, to landfill	2.77	lb	2.77	kg	
Solid Waste Sold for Recycling or Reuse	0.39	lb	0.39	kg	
Solid waste, process to incineration	0.10	lb	0.10	kg	
Hazardous waste to incineration	3.1E-04	lb	3.1E-04	kg	
Water Consumption	156	gal	1,300	l	

* To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by the order of magnitude of the average.

Source: Primary Data, 2018(e)

POLYETHYLENE TEREPHTHALATE (PET) MELT AND SOLID PHASE RESIN PRODUCTION

In this analysis, PET resin is only considered to be manufactured by the esterification of PTA with ethylene glycol and loss of water. No PET from dimethyl terephthalate (DMT) is considered in this dataset. PET from DMT are still used in North America for creating specialized products from PET, but these amounts are small compared to the use of PTA as a source for PET. The average data in this analysis includes PET resin manufactured using three technologies: melt phase and solid-state polymerization (SSP), melt-to-resin (MTR®) and Integrex®. Metals mining and processing for the catalysts have been included as an order of magnitude to protect confidentiality. A simplified description of each technology used is provided below.

The ethylene glycol inputs for these processes are a combination of monoethylene glycol (MEG) and diethylene glycol (DEG), which are created as coproducts and have similar LCA profiles. The amounts of MEG and DEG are fed at levels that vary with reactor design and operation. No LCI data was available for Isophthalic acid; therefore, PTA was used as a surrogate.

Most commonly, melt phase and solid-state polymerization is used to manufacture PET resin. This process requires two polymerization steps. The first polymerization step, the melt phase polymerization, is the esterification of ethylene glycol and PTA yielding a loss of water under high pressure and temperature. This step produces a low intrinsic viscosity PET pellets suitable for making clothing. A second polymerization step, solid-state polymerization, is used to achieve bottle-grade PET. This step raises the temperature of the solid pellets in the absence of oxygen and water. Polymer chains lengthen by using vacuum or inert gas. Temperature, pressure and the diffusion of by-products from inside the pellet are key to accomplishing SSP.

Melt-to-Resin (MTR®) technology is used by one of the data providers. In addition to ethylene glycol and purified terephthalic acid feedstocks, isophthalic acid and other additives are used in a melt phase polymerization. This technology uses a 2-reactor process that produces a resin with a high intrinsic viscosity, making it unnecessary to undergo additional steps required by solid state polymerization.

The patented Integrex® technology is used in one data provider producing PET resin. This technology differs from the other technologies used in the stage from the paraxylene feeding, through the production of PET. This technology integrates the paraxylene-to-PTA and PTA-to-PET steps, which were separated for this analysis to create horizontal averages of each unit process.

LCI data for the production of PET resin were collected from three producers (seven plants) in North America – all in the United States. All companies provided data for the year 2015. The captured production amount is approximately 50 percent of the available capacity for all PET resin production in North America in 2015. Small amounts (less than 1 percent of total output) of off-spec/trim/scrap resin are produced as coproducts during this process. A mass basis was used to allocate the credit for the coproduct. The average TPA/PTA and PET datasets were reviewed and accepted respectively by each TPA/PTA and PET data provider.

To assess the quality of the data collected for PET from PTA, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for PET include direct measurements, information provided by purchasing and utility records, and estimates. The technology represented by the PET data includes melt phase and solid-state polymerization (SSP), melt-to-resin (MTR®) and Integrex®.

Table 36 shows the average energy usage and environmental emissions for the for production of 1,000 pounds and 1,000 kilograms of PET using the three types of technologies. To indicate known emissions while protecting the confidentiality of individual company responses, some emissions are reported only by the order of magnitude of the average.

Table 36. Data for the Production of Polyethylene terephthalate (PET) Resin

	1,000 lb		1,000 kg		
Material Inputs					
Ethylene Glycol	345	lb	345	kg	
Purified Terephthalic Acid (PTA)*	838	lb	838	kg	
Isophthalic Acid*	22.4	lb	22.4	kg	
Catalyst metals included:					
Antimony	0.10	lb	0.10	kg	**
Cobalt	0.010	lb	0.010	kg	**
Titanium	0.10	lb	0.10	kg	**
Energy					
Process Energy					
Electricity from grid	104	kWh	230	kWh	
Natural gas	993	ft^3	62.0	m^3	
Coal	0.87	lb	0.87	kg	
Diesel	0.0030	gal	2.5E-05	m^3	
Residual Oil	0.0012	gal	9.8E-06	m^3	
Energy Credit					
Energy Credit from waste-to-energy	6,879	Btu	16.0	MJ	
Transportation Energy					
Barge	40.4	ton·mi	130	tonne·km	
Ship	475	ton·mi	1,530	tonne·km	
Pipeline	0.075	ton·mi	0.24	tonne·km	
Rail	103	ton·mi	330	tonne·km	
Truck	5.90	ton·mi	19.0	tonne·km	
Environmental Emissions					
Atmospheric Emissions					
Aldehydes, unspecified	0.0010	lb	0.0010	kg	**
Particulates, unspecified	0.010	lb	0.010	kg	**
Particulates, > 2.5 um, and < 10um	0.0062	lb	0.0062	kg	
Particulates, < 2.5 um	0.022	lb	0.022	kg	
Hydrocarbons, unspecified	0.010	lb	0.010	kg	**
Ammonia	0.0010	lb	0.0010	kg	**
Dioxane, 1,4-	0.0010	lb	0.0010	kg	**
Diphenyl ether	1.0E-05	lb	1.0E-05	kg	**
Furan	1.0E-05	lb	1.0E-05	kg	**
Toluene	0.0010	lb	0.0010	kg	**
Xylene	1.0E-05	lb	1.0E-05	kg	**
Biphenyl	0.0010	lb	0.0010	kg	
Ethylene glycol	0.049	lb	0.049	kg	**
Acetaldehyde	0.010	lb	0.010	kg	**

Table 36. Data for the Production of Polyethylene terephthalate (PET) Resin (continued)

	1,000 lb		1,000 kg		
Environmental Emissions					
Waterborne Releases					
Fluoride	1.0E-04	lb	1.0E-04	kg	**
BOD5, Biological Oxygen Demand	0.11	lb	0.11	kg	
COD, Chemical Oxygen Demand	0.57	lb	0.57	kg	
Phenol	1.0E-06	lb	1.0E-06	kg	**
Oils, unspecified	0.0010	lb	0.0010	kg	**
Suspended solids, unspecified	0.010	lb	0.010	kg	**
Cyanide	1.0E-06	lb	1.0E-06	kg	**
Iron	0.010	lb	0.010	kg	**
Aluminium	0.0010	lb	0.0010	kg	**
Nickel	1.0E-06	lb	1.0E-06	kg	**
Lead	1.0E-08	lb	1.0E-08	kg	**
Phosphate	0.0010	lb	0.0010	kg	**
Zinc	1.0E-05	lb	1.0E-05	kg	**
Ammonia	0.0010	lb	0.0010	kg	**
Sulfate	0.10	lb	0.10	kg	**
Magnesium	0.010	lb	0.010	kg	**
Nitrate	0.0010	lb	0.0010	kg	**
Bromide	0.0010	lb	0.0010	kg	**
Nitrogen, total	0.0010	lb	0.0010	kg	**
Antimony	1.0E-04	lb	1.0E-04	kg	**
1,4-Dioxane	0.010	lb	0.010	kg	**
Acetaldehyde	0.010	lb	0.010	kg	**
Ethylene glycol	0.10	lb	0.10	kg	**
2-methyl-1,3-dioxolane	0.0010	lb	0.0010	kg	**
Solid Wastes					
Non-hazardous waste to landfill	0.47	lb	0.47	kg	
Non-hazardous waste, recovery	0.77	lb	0.77	kg	
Non-hazardous waste to incineration	0.0034	lb	0.0034	kg	
Non-hazardous waste to WTE	0.68	lb	0.68	kg	
Hazardous waste to incineration	0.0048	lb	0.0048	kg	
Water Consumption	87.4	gal	730	l	

* An LCI dataset was not available for Isophthalic acid, so PTA was used as a surrogate for this chemical.

** To indicate known input/emissions while protecting the confidentiality of individual company responses, the input/emission is reported only by the order of magnitude of the average.

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Primary data was collected from seven plants from three leading PET manufacturers.

Source: Primary data, 2018(f).

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