CRADLE-TO-GATE LIFE CYCLE ANALYSIS OF TOLUENE DIISOCYANATE (TDI)

Final Report

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Submitted by:

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PREFACE

This life cycle assessment of Toluene Diisocyanate (TDI) was commissioned and funded by the American Chemistry Council (ACC) Plastics Division to update the original data in the 2011 report, **Cradle-to-Gate Life Cycle Inventory of Nine Plastic Resins and Four Polyurethane Precursors**, as well as the U.S. LCI plastics database. The report was made possible through the cooperation of ACC member companies, who provided data used in this report.

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

Franklin Associates gratefully acknowledges the significant contribution to this project by Allison Chertack, Prapti Muhuri, Mike Levy (First Environment Inc., formerly ACC), and Keith Christman in leading this project. We gratefully acknowledge the contribution of BASF in providing data that were used to validate the previously collected data for modeling TDI production.

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

May, 2023

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LIST OF ACRONYMS

(Alphabetical)

ACC	AMERICAN CHEMISTRY COUNCIL
AP	ACIDIFICATION POTENTIAL
API	AMERICAN PETROLEUM INSTITUTE
BOD	BIOCHEMICAL OXYGEN DEMAND
BTEX	BENZENE, TOLUENE, ETHYLBENZENE, AND XYLENE
COD	CHEMICAL OXYGEN DEMAND
CFC	CHLOROFLUOROCARBON
DNT	DINITROTOLUENE
EGRID	EMISSIONS & GENERATION RESOURCE INTEGRATED DATABASE
EIA	ENERGY INFORMATION ADMINISTRATION
EP	EUTROPHICATION POTENTIAL
ERG	EASTERN RESEARCH GROUP, INC
EQ	EQUIVALENTS
EU	EUROPEAN UNION
GHG	GREENHOUSE GAS
GHGRP	GREENHOUSE GAS REPORTING PROGRAM
GJ	GIGAJOULE
GREET	GREENHOUSE GASES, REGULATED EMISSIONS, AND ENERGY USE IN TECHNOLOGIES
GWP	GLOBAL WARMING POTENTIAL
HCFC	HYDROCHLOROFLUOROCARBON
IPCC	INTERGOVERNMENTAL PANEL ON CLIMATE CHANGE
ISO	INTERNATIONAL ORGANIZATION FOR STANDARDIZATION
ISOPA	EUROPEAN DIISOCYANATE AND POLYOL PRODUCERS ASSOCIATION
LCA	LIFE CYCLE ASSESSMENT
LCI	LIFE CYCLE INVENTORY
LCIA	LIFE CYCLE IMPACT ASSESSMENT
LPG	LIQUEFIED PETROLEUM GAS

MJ	MEGAJOULE
MM	MILLION
NAICS	NORTH AMERICAN INDUSTRY CLASSIFICATION SYSTEM
NAPAP	NATIONAL ACID PRECIPITATION ASSESSMENT PROGRAM
NGL	NATURAL GAS LIQUID
NMVOC	NON-METHANE VOLATILE ORGANIC COMPOUNDS
NREL	NATIONAL RENEWABLE ENERGY LABORATORY
ODP	OZONE DEPLETION POTENTIAL
POCP	PHOTOCHEMICAL SMOG FORMATION (HISTORICALLY PHOTOCHEMICAL OXIDANT CREATION POTENTIAL)
RCRA	RESOURCE CONSERVATION AND RECOVERY ACT
SI	INTERNATIONAL SYSTEM OF UNITS
TDA	TOLUENE DIAMINE
TDI	TOLUENE DIISOCYANATE
TRACI	TOOL FOR THE REDUCTION AND ASSESSMENT OF CHEMICAL AND OTHER ENVIRONMENTAL IMPACTS
TRI	TOXIC RELEASE INVENTORY
WTE	WASTE-TO-ENERGY INCINERATION

CRADLE-TO-GATE LIFE CYCLE ASSESSMENT OF TOLUENE DIISOCYANATE (TDI)

INTRODUCTION

This study provides the American Chemistry Council (ACC), their members, users of the U.S. LCI Database, and the public at large with information about the life cycle inventory and impacts for the production of Toluene Diisocyanate (TDI), which is a precursor in the manufacture of flexible polyurethane foams that are used for carpet pads, furniture, bedding, and packaging applications. TDI is also used to produce polyurethanes used in elastomers, coatings, sealants and adhesives.[1] 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.

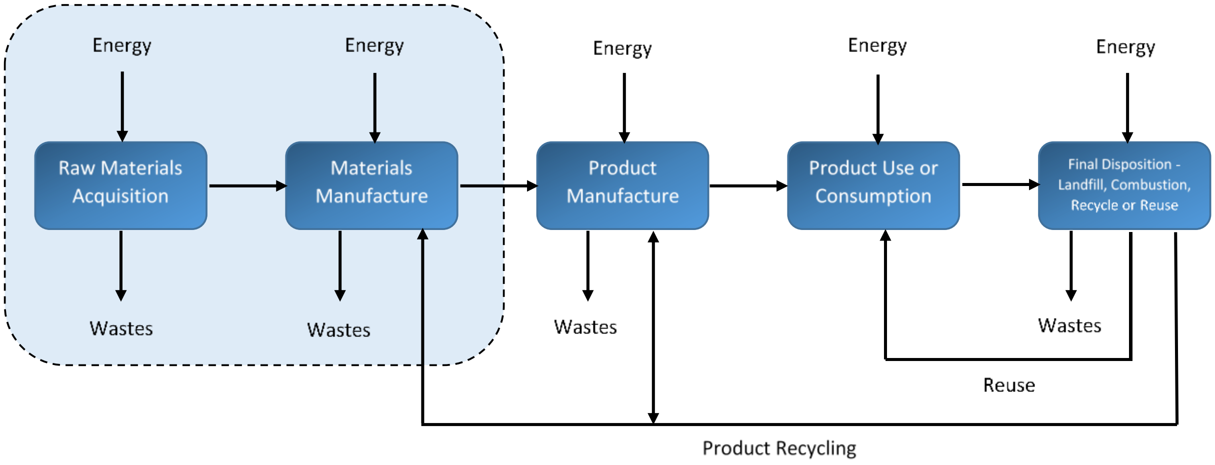

Figure 1. General materials flow for "cradle-to-grave" analysis of a product system. The dashed box indicates the boundaries of this analysis.

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.

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[1] From the website: https://www.diisocyanates.org/about-institute

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 TDI. It is considered a cradle-to-gate boundary system because this analysis ends with the TDI production. The system boundaries stop at the TDI production so that the data can be linked to a fabrication process where it is an input material, and end-of-life data to create full life cycle inventories for a variety of applications, such as injection molded products, cushions, and sealants. The method used for this inventory has been conducted following internationally accepted standards for LCI and LCA methodology as outlined in the International Organization for Standardization (ISO) 14040:2006 and 14044:2006 standard documents[2].

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 aggregated LCI data for the phosgene/DNT/TDA/TDI unit process is shown separately in the attached Appendix. Because less than three TDI manufacturers were available to provide data for this analysis, the average 2003 TDI data collected for the previous 2011 study were used with some updates to input materials and intermediate chemicals. The LCI data for crude oil and natural gas is shown in the appendix of a separate report, Cradle-to-Gate Life Cycle Analysis of Olefins[3]. Discussion of LCI data for ammonia, nitric acid and carbon monoxide is available in a separate report, Cradle-to-Gate Life Cycle Analysis of Methylene Diphenyl Diisocyanate (MDI)[4]. Primary LCI data for chlorine and sodium hydroxide are discussed in a separate report, Cradle-to-Gate Life Cycle Analysis of Polyvinyl Chloride (PVC) Resin[5]. All unit processes are either available currently or will be made available to the National Renewable Energy Laboratory (NREL) who maintains the U.S. LCI Database.

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[2] 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.

[3] Cradle-to-Gate Life Cycle Analysis of Olefins. Franklin Associates. Submitted to the Plastics Division of the American Chemistry Council. April, 2020.

[4] Cradle-to-Gate Life Cycle Analysis of Methylene Diphenyl Diisocyanate (MDI). Franklin Associates. Submitted to the Plastics Division of the American Chemistry Council. July, 2022.

[5] Cradle-to-Gate Life Cycle Analysis of Polyvinyl Chloride (PVC) Resin. Franklin Associates. Submitted to the Plastics Division of the American Chemistry Council. December, 2021.

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.

STUDY GOAL AND INTENDED USE

The purpose of this LCA is to document the LCI data and then evaluate the environmental profile of TDI. 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 TDI; and
- To provide information about the environmental burdens associated with the production of TDI. The LCA results for TDI production can be used as a benchmark for evaluating future updated TDI results for North America.

According to ISO 14040:2006 and 14044:2006 standards, a critical or peer review is not required as no comparative assertions of competing materials or products are made in this study.

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FUNCTIONAL UNIT

The function of TDI is primarily for use as a polyurethane precursor. Industries that use polyurethanes with TDI as a precursor include furniture, bedding, and carpet manufacturers. As the study boundary concludes at the TDI, a mass functional unit has been chosen. Results for this analysis are shown on a basis of both 1,000 pounds and 1,000 kilograms of TDI produced.

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 TDI manufacture:

- Raw material extraction (e.g., extraction of petroleum and natural gas as feedstocks) through toluene, nitric acid, carbon monoxide, chlorine, and sodium hydroxide production and incoming transportation for each process, and
- TDI manufacture, which is aggregated with phosgene, dinitrotoluene (DNT), and toluene diamine (TDA), including incoming transportation for each material.

This report includes LCI results, as well as LCIA results, for TDI manufacturing. Figure 2 presents the flow diagram for the production of TDI. A unit process description and tables for each box shown in the flow diagram can be found in the attached appendix, or in the previously released olefins, MDI, or the PVC resin report. Unit processes included within the dotted rectangle are included in an aggregated dataset.

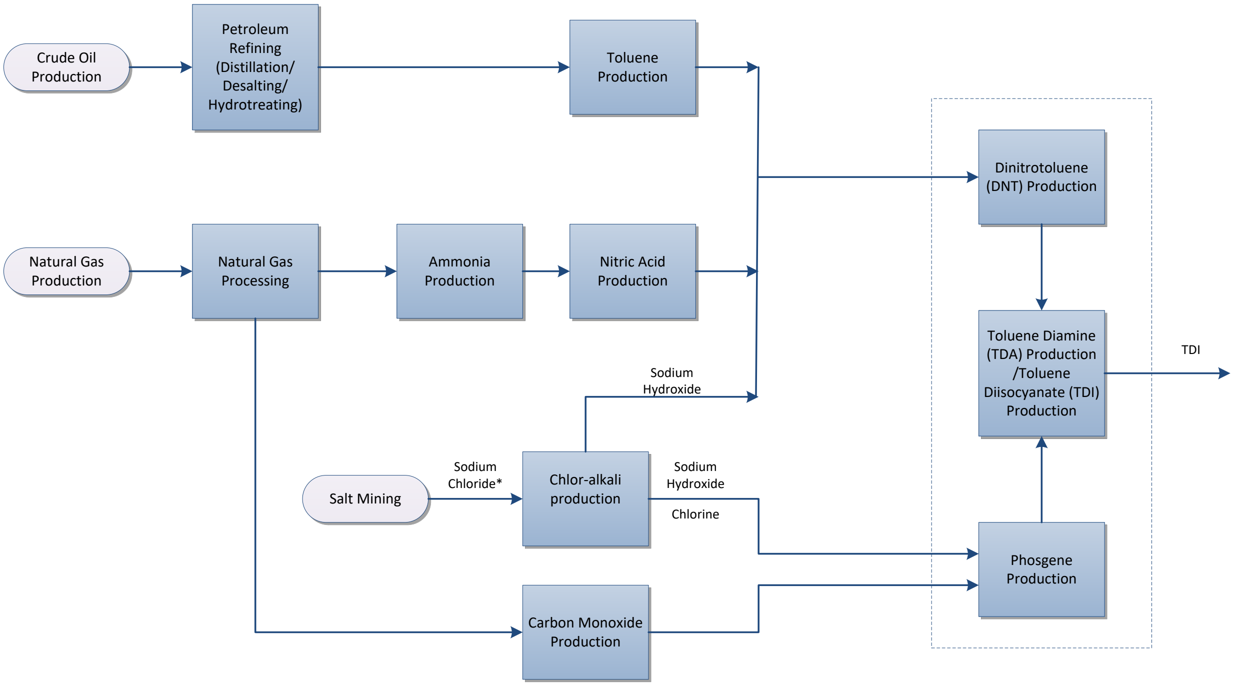

Figure 2. Flow diagram for the Production of Toluene Diisocyanate (TDI).
* Sodium chloride data are from ecoinvent and are adapted to U.S. conditions.

Technological Scope

The overall technology is similar in all plants of this analysis for producing TDI. Toluene diisocyanate is manufactured by first producing intermediate products; diamines (TDA) and phosgene. Diamines are produced from the dinitrotoluene reaction and phosgene is produced from carbon monoxide and chlorine gases. The intermediate products are then reacted to form a mixture of several TDI isomers. Purification of crude TDI is the final step in TDI manufacture.

Temporal and Geographic Scope

To assess the quality of the data collected for TDI, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for TDI include direct measurements, information provided by purchasing and utility records, and estimates. Data submitted for TDI represent the year 2003 and all production is in U.S. Because there are currently only two companies manufacturing TDI within North America, the average data from the previous 2011 study (2003 data) has been used with some changes to input materials and intermediate chemicals. Additionally, the manufacturing process used to produce TDI has not changed significantly since the last data collection effort in 2003. Three companies (three plants) provided data for the year 2003. Data for steam reforming was taken from primary European data from the 1990s, but adapted to U.S. conditions, and the energy was decreased for efficiency increases over time. Again, the steam reforming process has not significantly changed over the past 3 decades.

The geographic scope of the analysis is the manufacture of TDI in North America. All TDI data collected were from plants in the United States and some input materials were modeled using North American databases such as the U.S. LCI database, GREET, and Franklin Associates' private database, as well as ecoinvent. Datasets from ecoinvent or primary European data were adapted to U.S. conditions to the extent possible (e.g., by using U.S. average grid electricity to model production of process electricity reported in the European data sets). The U.S. electricity grid from 2016 was taken from information in Emissions & Generation Resource Integrated Database (eGRID) 2016 database.

Exclusions from the Scope

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, no use of resource-intensive or high-toxicity chemicals or additives was identified. Therefore, the results for TDI production are not expected to be understated by any significant amount due to substances that may be used in small amounts. Small amounts of sulfuric acid and soda ash were removed from the original study as they were within the 1 percent cut-off but included originally.

- **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 conduct 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 TDI 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.

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 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.[6] For the category of Global Warming Potential (GWP), contributing elementary flows are characterized using factors reported by the Intergovernmental Panel on Climate Change

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[6] 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.

(IPCC) in 2013 with a 100-year time horizon.[7] 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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[7] 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.	Million (MM) Btu and megajoule (MJ)	Cumulative energy inventory
	Non-renewable energy demand	Measures the fossil and nuclear energy from point of extraction.	MM Btu and MJ	Cumulative energy inventory
	Renewable energy demand	Measures the hydropower, solar, wind, and other renewables, including landfill gas use.	MM Btu and MJ	Cumulative energy inventory
	Solid waste by weight	Measures quantity of fuel and process waste to a specific fate (e.g., landfill, waste-to-energy (WTE)) for final disposal on a mass basis	Lb and 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 and 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 CO_2 equivalents (eq) and 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 SO_2 eq and 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, chemical oxygen demand (COD) and biochemical oxygen demand (BOD), N and P compounds	Lb N eq and kg N eq	TRACI v2.1
	Ozone depletion potential	Measures stratospheric ozone depletion. Important emissions: chlorofluorocarbon (CFC) compounds and halons	Lb CFC-11 eq and 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, benzene, toluene, ethylbenzene, xylene (BTEX), non-methane volatile organic compound (NMVOC), CH_4, C_2H_6, C_4H_{10}, C_3H_8, C_6H_{14}, acetylene, Et-OH, formaldehyde	Lb kg O_3 eq and kg O_3 eq	TRACI v2.1

DATA SOURCES

The purpose of this study is to update the life cycle profile for TDI using the most recent data available for each process. Due to a lack of TDI manufacturers within North America to provide primary TDI data for this analysis, the average 2003 TDI data from the original study was reviewed and compared to a 2015 updated TDI dataset. The method for allocation of energy sold from the process was updated to system expansion and incoming transportation updated as necessary. A weighted average was calculated for the TDI data collected for this analysis from the year 2003. Primary data was collected for the chlor-alkali process. Primary data from the 1990s was reviewed, adapted, and used for the steam reforming portion of toluene. The toluene data were adapted to US conditions (e.g., replacement of oil fuels with natural gas, transportation estimated for US), and the energy was decreased for efficiency increases over time. Secondary source data was researched in 2017 for crude oil extraction and refining and natural gas production and processing. Secondary sources were used for sodium chloride (brine), ammonia, nitric acid, and carbon monoxide production. All included processes are shown in the appendix at the end of the report or within a previously released report. All included processes are shown in Figure 2.

LCI data for the production of TDI were collected from three producers (three plants) in North America – all in the United States. All companies provided data from the year 2003. A weighted average was calculated from the data collected and used to develop the LCA model. Weightings were not updated from 2003 as one plant has closed and one has been sold. Hydrochloric acid is a coproduct of TDI production, and for the results discussed in this report, a mass basis was used to allocate all inputs and outputs between the coproducts (See Coproduct Allocation for more information).

LCI data for the chlor-alkali process were collected from three producers (three plants) using the membrane technology in the United States. Two of the plants provided data for the year 2015, while one provided data for the year 2017. A weighted average was calculated from the data collected and used to develop the LCA model. A combination of stoichiometric and mass allocation was used for the chlorine, sodium hydroxide, and hydrogen coproducts from this process. Stoichiometric allocation was used for the material inputs, while mass allocation was used for all other inputs and outputs. This follows the same method used by PlasticsEurope for their chlor-alkali process LCA. Small amounts of hydrogen were considered a coproduct at the plants. In some cases, much of the hydrogen created was used as a fuel in the chlor-alkali or down-stream PVC processes or it was used to make hydrochloric acid on-site.

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 TDI is 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 provided TDI data from 2003 and one company provided 2015 data, which were compared to the older average data and found to be comparable and still geographically representative data for all primary TDI data collected for this LCA.

Most of the incoming material and fuel datasets for TDI manufacture were either updated using geographical and technologically relevant data from government or privately available statistics/studies within the US or drawn from either The Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) Model or ecoinvent[8],[9]. The toluene data was a 70/30 percent split between steam reforming and pyrolysis gasoline, which included primary European steam reforming data from the 1990s, which was reviewed and adapted to U.S. conditions (including conversion of oil fuels used in on-site boilers to natural gas). The steam reforming technology has not changed significantly over the past three decades. Datasets from ecoinvent and primary European datasets were adapted to U.S. conditions to the extent possible (e.g., by using U.S. average grid electricity to model production of process electricity reported in the European data sets). 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 collected. All primary data obtained specifically for this study were considered the most representative available for the systems studied. Although data for toluene and TDI come from older sources, the overall technology used to produce these chemicals has remained overall the same since the data was collected. 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.

Representativeness: TDI manufactured in North America is representative of the majority of TDI producers within the United States. The three companies provided data from their facilities using technology ranging from average to state-of-the-art. After reviewing individual company data in comparison to the average, each manufacturer verified the average data from 2003 was a representative for TDI production in North America. The chlorine/caustic data collected for this module represent three producers and three plants in the U.S. In 2002, there were five TDI producers and six TDI plants in the U.S. Currently, there are two TDI manufacturers in North America.

LCI data from the sources of input materials specific to each company providing data was not available for this analysis. As impacts from crude oil and natural gas may vary depending

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[8] Argonne National Laboratory, Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies Model; Energy Systems Division, https://greet.es.anl.gov/, 2017, accessed August 1, 2018.

[9] 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].

on transportation requirements some variability in data and impact on LCA results should be expected.

The average TDI unit process data was based on the best available U.S. data at the time the study was conducted. As in all LCA studies, the ability to develop a representative average is determined by the number of companies willing to participate. Data from this analysis was used to develop the most representative average for TDI production, which happened to be in the 2003 time frame. It should be noted that one company did provide updated 2015 data, which was used as a comparison to the older data average. Overall, the differences in the 2003 and 2015 data received were a small amount lower for the fuels used. Emissions varied by small amounts both higher and lower than the previous average.

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.

Order of Magnitude: In some cases, emissions data were reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only as an order of magnitude. An order of magnitude of a number is the smallest power of 10 used to represent that number. For example, if the average of two data points for a particular emission is 2.5E-4, the amount would be shown as 1.0E-4 to ensure confidentiality of the data providers but allow the impact assessment tool to include a close estimate of the amount within any pertinent impact categories. When order of magnitude is used in the LCI data shown in the Appendix of this report, it is clearly noted by an asterisk next to the amount.

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, 2003 primary data were used to model the phosgene/DNT/TDA/TDI, while current primary data was used to model the chlor-alkali process. 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, GREET, and ecoinvent.

A report from the International Energy Agency (IEA) that at this time has not been subject to validation through a scientific peer review suggests that unwanted methane emissions during oil and gas extraction, processing and transport are higher than assumed in current LCA databases. The IEA has created a methane tracker website reporting these additional methane emissions[10]. As a base case, the present U.S. cradle-to-gate reports use oil and gas extraction information published by the National Energy Technology Laboratory (NETL), Argonne National Laboratory (ANL), and the Energy Information Administration (EIA), which currently do not include these increased methane losses.

METHOD

The LCA has been conducted following internationally accepted standards for LCA as outlined in the ISO 14040:2006 and 14044:2006 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 olefins produced at the 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 off-gas 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

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[10] IEA (2020), Methane Tracker 2020, IEA, Paris https://www.iea.org/reports/methane-tracker-2020

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.

Environmental burdens are allocated among the coproducts 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 allocating the environmental burdens among the coproducts 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 the "upstream" chemical process involved in producing TDI, chlor-alkali, and olefins.

Franklin Associates follows the guidelines for allocating the environmental burdens among the coproducts as shown in the ISO 14044:2006 standard on life cycle assessment requirements and guidelines[11]. 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.

Rationale for Choice of Allocation Method for TDI/HCl Coproducts in North America

In the case of North American isocyanate (MDI and TDI) production, Franklin Associates used a mass allocation for the original isocyanates/HCl coproduct allocation as discussed in the 2011 report. For this TDI report, results using mass allocation for TDI/HCl are provided in the results section. Recently, the European Diisocyanate and Polyol Producers Association (ISOPA) released a new dataset for TDI and TDI for European manufacturers that uses a combined elemental and mass allocation[12]. At the release of this report in July 2022, the ISOPA report is final and uses this new method. A sensitivity analysis was provided in the ISOPA report showing results for both mass and the combined allocation methods. Thus, to be consistent, a sensitivity analysis providing both allocation methods is presented in this North American report. The results using a mass allocation allow the reader to compare to the original 2011 TDI results; while the results using combined elemental and mass allocation allow the reader to compare the current North American TDI results to the current EU TDI results. The most recent round of discussions on the product environmental footprint of isocyanates have been concluded in Europe and led to mutual acceptance of this allocation method by EU producers of MDI/TDI and ISOPA. Moving forward, the ACC will continue to work in partnership with the producers of MDI/TDI and engage with ISOPA to discuss any

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

[12] ISOPA Eco-profile of toluene diisocyanate (TDI) and methylene diphenyl diisocyanate (TDI). April 2021.

further decisions made by ISOPA in collaboration with the EU government concerning LCA methodologies and approaches to ensure consistency as much as possible.

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. If system expansion is not possible, 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 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 primary TDI production. The material coproducts from pyrolysis gasoline production for all plants included propylene, ethylene, butadiene, ethane, hydrogen, acetylene, crude benzene, and small amounts of various heavy end products. In the chlor-alkali plant, allocations have been made to focus on which product the inputs or outputs associate within the process. The specifics of the allocations given in the chlor-alkali plants are detailed in the report, *Cradle-to-gate Life Cycle Analysis of Polyvinyl Chloride (PVC) Resin*.[13] The material coproduct from TDI production includes a sizable amount of hydrochloric acid. The results discussed in this report are based on the TDI unit processing using mass allocation. However, a sensitivity analysis using the elemental and mass allocation has been included. An explanation of this allocation is provided in the sensitivity analysis section.

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

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[13] Cradle-to-Gate Life Cycle Analysis of Polyvinyl Chloride (PVC) Resin. Franklin Associates. Submitted to the Plastics Division of the American Chemistry Council. December, 2021.

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.

Elemental/Mass Coproduct Allocation in Sensitivity Analysis

In 2021, ISOPA released their updated MDI/TDI Eco-profile, which used an allocation method combining elemental and mass allocation. For this analysis, the elemental + mass allocation method has been applied to both the current TDI and original TDI data in a sensitivity analysis. For this allocation, the following allocations are given using the elemental + mass allocation:

- The chlorine input is fully allocated to the production of HCl.
- The inputs used to create TDI and phosgene/DNT/TDA are fully allocated to TDI.
- Chlorine or Hydrochloric acid atmospheric emissions or waterborne releases are fully allocated to the HCl.
- All other inputs/outputs have been given mass allocation.

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 Emissions & Generation Resource Integrated Database (eGRID) 2016 database[14].

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.

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

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 2016 industry statistics, natural gas accounted for 75 percent of industrial cogeneration, while coal and biomass accounted for the largest portion of the remaining fuels used[15].

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.

   The 50 percent conversion efficiency was an estimate after reviewing EIA fuel consumption and electricity net generation data from cogeneration plants in 2016.[16] The straight average conversion efficiency for 2016 for electricity production in cogeneration plants within this database is a little more than 55 percent; however, the range of efficiency calculated per individual cogeneration plant was 23% to 87%. The 50 percent estimate of conversion efficiency was used previously in the 2011 database and so was estimated for continued use within this analysis, due to the variability of the individual cogeneration plants. Unit process data for cogeneration of electricity is provided by kWh, so that a change of efficiency could easily be applied during modeling.

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

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[15] U.S. Department of Energy. *Combined Heat and Power (CHP) Technical Potential in the United States.* March 2016.

[16] U.S. Department of Energy, The Energy Information Administration (EIA). *EIA-923 Monthly Generation and Fuel Consumption Time Series File, 2016 Final Revision*

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[17]. This Btu value was then divided by the Btu value of fuel consumed in the cogeneration boiler to determine the steam allocation factor. In 2015, the 80 percent efficiency used is common for a conventional natural gas boiler, which should not change when considering the steam portion of the cogeneration system. Pounds of steam, temperature and pressure were provided by participating plants. Steam tables were used to calculate energy amounts, which was divided by the efficiency and converted to natural gas amounts in cubic feet.

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[17] United States Environmental Protection Agency (EPA). *Methods for Calculating CHP Efficiency*. Accessed online at https://www.epa.gov/chp/methods-calculating-chp-efficiency.

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 TDI:

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 unit processes, for TDI:

- Cradle-to-incoming materials – includes the raw materials through the production of carbon monoxide, toluene, nitric acid, chlorine, and sodium hydroxide (inputs to the phosgene/DNT/TDA/TDI processes)
- TDI production – is the gate-to-gate unit process and includes the production of fuels used in the processes to create phosgene/DNT/TDA/TDI. Within the discussion, the aggregated unit processes for phosgene/DNT/TDA/TDI will be called TDI production or unit process.

Tables and figures are provided for TDI in each inventory and impact category section in this report. The phrases “cradle-to- “and “system” are defined as including all of the raw and intermediate chemicals required for the production of the chemical stated in the term (e.g., cradle-to-TDI and TDI system are interchangeable). The phrase “gate-to-gate” is defined as including only the onsite process/fuels/nitrogen for the unit process.

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 most of the incoming chemicals (e.g., the energy content of oil and gas used as material feedstocks) to the phosgene/DNT/TDA/TDI.

The average total energy required to produce TDI is 19.8 million Btu per 1,000 pounds of TDI or 46.2 GJ per 1,000 kilograms of TDI. Table 2 shows total energy demand for the life cycle of TDI production. The TDI production energy has been split out from the energy required for incoming materials. Twenty-five percent of the total energy is required to produce the TDI, but this does include a number of incoming materials to the TDI process in order to conceal confidential information. The remaining 75 percent is used to create the incoming materials and their raw materials.

Table 2. Total Energy Demand for TDI

	Basis: 1,000 pounds		
	Total Energy	**Non-Renewable Energy**	**Renewable Energy**
	MM Btu	***MM Btu***	***MM Btu***
Cradle-to-Incoming Materials	14.8	14.7	0.11
DNT/Phosgene/TDA/TDI Production	5.01	4.99	0.018
Total	**19.8**	**19.7**	**0.13**
	Basis: 1,000 kilograms		
	Total Energy	**Non-Renewable Energy**	**Renewable Energy**
	GJ	***GJ***	***GJ***
Cradle-to-Incoming Materials	34.5	34.2	0.26
DNT/Phosgene/TDA/TDI Production	11.7	11.6	0.042
Total	**46.2**	**45.9**	**0.30**
	Percentage		
	Total Energy	**Non-Renewable Energy**	**Renewable Energy**
	%	***%***	***%***
Cradle-to-Incoming Materials	74.7%	74.2%	0.56%
DNT/Phosgene/TDA/TDI Production	25.3%	25.2%	0.09%
Total	**100%**	**99.4%**	**0.65%**

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), as well as use of uranium to generate the share of nuclear energy in the average U.S. kWh. For TDI, 99.4 percent of the total energy comes from non-renewable sources. The renewable energy demand consists of electricity derived from renewable energy sources (primarily hydropower, as well as wind, solar, and other sources). The renewable energy (0.04 GJ/1000 kg) used at the TDI plant comes solely from hydropower and other renewable sources (geothermal, solar, etc.) from electricity production.

The energy representing natural gas and petroleum used as raw material inputs for the production of incoming chemicals used to produce TDI are included in the cradle-to-incoming material amounts in Table 2. The energy inherent in these raw materials are called material feedstock energy. Of the total energy (46.2 GJ) for 1,000 kg of TDI, 23 GJ is material feedstock energy. Figure 3 provides the breakdown of the percentage of total energy required for material feedstock energy versus the process and fuel energy amounts needed to produce the TDI. Approximately 50 percent of the total energy is inherent energy in the natural gas and petroleum used as a feedstock to create chemicals such as carbon monoxide and toluene, which in turn are used to create TDI. Of the feedstock sources for TDI, 45 percent come from oil, while 55 percent of the feedstock sources come from natural gas. The toluene technology was chosen as 70 percent from steam reforming (oil-based) and 30 percent from pygas (mostly natural gas-based); if this assumption was changed to a different mix of steam reforming, pyrolysis gas, and other types of technology used to produce toluene, the split of feedstock sources would change.

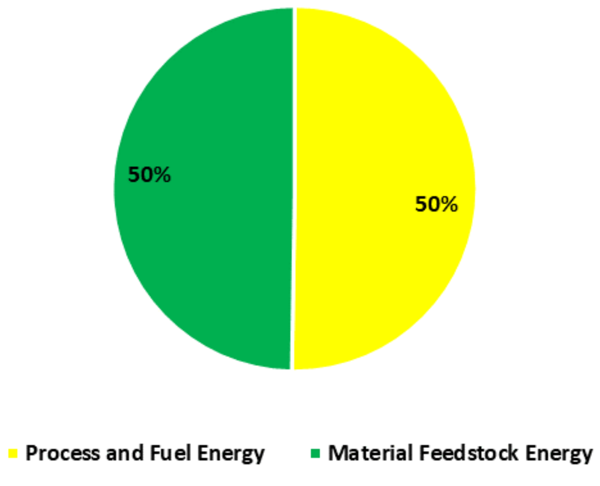

Figure 3. Process/Fuel and Material Feedstock Percentages for TDI

Energy Demand by Fuel Type

The total energy demand by fuel type for TDI is shown in Table 3 and the percentage mix is shown in Figure 4. Natural gas and petroleum together make up over 92 percent of the total energy used. As shown in Figure 3, this is partially due to the material feedstock energy used to create the incoming chemicals to TDI. These material feedstock fuels are part of the energy shown in the natural gas and petroleum split out in the following table and figure. The gate-to-gate production energy for TDI in the following table and figure represents the energy required for transportation of raw materials to the plants, the energy required to produce the direct incoming chemicals (phosgene, DNT, TDA) and the TDI output, and the production of the fuels needed to manufacture the immediate incoming chemicals and TDI.

Petroleum-based fuels (e.g., diesel fuel) are the dominant energy source for transportation. Natural gas, coal, and other fuel types, such as hydropower, nuclear and other (geothermal, wind, etc.) are used to generate purchased electricity.

Of the results for TDI production shown in Table 3 and Figure 4, almost 70 percent of the energy used (32.3 GJ/46.2 GJ) is from natural gas. At the TDI plant, over 95 percent of the energy used (11.2 GJ/11.7 GJ) comes from natural gas. Of the natural gas used at the TDI plant, 85 percent is combusted on-site, while 15 percent is required to create electricity either through the grid or through a nearby cogeneration plant. Petroleum comprises 23 percent (10.6 GJ/46.2 GJ) of the fuel types used for the TDI production system. The largest portion of petroleum is used for the production of toluene as a material input. The petroleum for the TDI plant is only 0.1 percent of the total and is used to create electricity and for transport. The coal use shown is combusted for electricity use. The 2016 U.S. electricity grid is used for this study. In this grid, approximately 30 percent of the electricity production in the US uses coal as a fuel source, while a third of the grid comes from natural gas and 20 percent from uranium. The hydropower, nuclear, and other energy are all used to create electricity.

Table 3. Energy Demand by Fuel Type for TDI

	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-Incoming Materials	14.8	9.07	4.54	0.67	0.45	0.047	0.063
DNT/Phosgene/TDA/TDI Production	5.01	4.80	0.012	0.11	0.072	0.0076	0.011
Total	**19.8**	**13.9**	**4.55**	**0.77**	**0.52**	**0.055**	**0.073**
	Basis: 1,000 kilograms						
	Total Energy	**Natural Gas**	**Petroleum**	**Coal**	**Nuclear**	**Hydropower**	**Other Renewable**
	GJ	***GJ***	***GJ***	***GJ***	***GJ***	***GJ***	***GJ***
Cradle-to-Incoming Materials	34.5	21.1	10.6	1.55	1.04	0.11	0.15
DNT/Phosgene/TDA/TDI Production	11.7	11.2	0.027	0.25	0.17	0.018	0.025
Total	**46.2**	**32.3**	**10.6**	**1.79**	**1.21**	**0.13**	**0.17**
	Percentage of Total						
	Total Energy	**Natural Gas**	**Petroleum**	**Coal**	**Nuclear**	**Hydropower**	**Other Renewable**
	%	***%***	***%***	***%***	***%***	***%***	***%***
Cradle-to-Incoming Materials	74.7%	45.7%	22.9%	3.4%	2.3%	0.24%	0.32%
DNT/Phosgene/TDA/TDI Production	25.3%	24.2%	0.1%	0.5%	0.4%	0.04%	0.05%
Total	**100%**	**69.9%**	**22.9%**	**3.9%**	**2.6%**	**0.28%**	**0.37%**

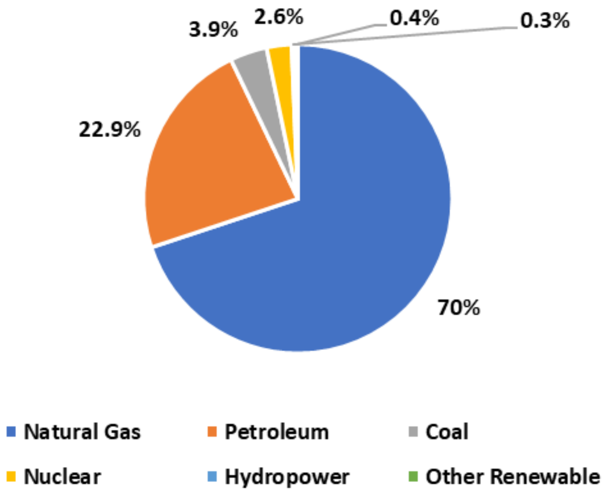

Figure 4. Percentage of Energy Separated by Fuel Type for TDI

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 the olefins (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 TDI are included in this analysis as no product is made from the material in the analysis boundaries.

The process solid waste, those wastes produced directly from the production of materials, includes wastes that are incinerated both for disposal and for waste-to-energy, as well as landfilled. Some wastes that are recycled/reused or land applied are not included as solid wastes, and no credit is given. The categories of disposal type 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 for the TDI system are shown in Table 4 and Figure 5. The solid wastes have been separated into hazardous and non-hazardous waste categories, as well as by the cradle-to-incoming materials and the TDI plant. Overall, the TDI plant produces the greatest amount of total solid waste at 37 percent, which is mostly hazardous waste. The solid waste associated with coal extraction and combustion to create electricity make up over 33 percent of the total solid waste. The extraction and processing of oil and gas used as a material and as a fuel creates 28 percent of the total solid waste.

As shown in Figure 5, 48 percent of the total solid waste is created during the TDI unit process. More than three-quarters of this amount comes from process solid wastes at the plant, while the remainder of the solid waste for TDI production comes from natural gas combustion at the plant and fuels combusted for the electricity used in the plant. The larger portion of solid waste, 52 percent, comes from the production of incoming materials used to produce phosgene/DNT/TDA/TDI. Approximately 23 percent of the total solid waste comes from the cradle-to-chlorine/sodium hydroxide production with another 18 percent coming from the cradle-to-toluene production.

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. 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. No solid wastes were stated as hazardous in the data sources for oil and gas. Hazardous waste comprises 35 percent of the total solid waste. Over 99 percent of the hazardous waste comes from the TDI plant, with less than 1 percent from pygas plants used to create toluene. No hazardous wastes are released at the chlor-alkali plants, which were primary data. It is possible that some hazardous wastes are overlooked during the steam reforming of toluene (70% of the toluene technology assumed).

Table 4 also provides a breakout of the total solid wastes by the disposal fate. Of the hazardous waste, almost 100 percent is used for waste-to-energy, while small amounts are sent to landfill and incineration. Focusing specifically on the non-hazardous solid waste produced, more than 99 percent of the non-hazardous solid waste is landfilled. Much of the data used for the incoming materials comes from secondary sources, so if no fate was provided for solid waste, landfilling was assumed.

Table 4. Total Solid Wastes for TDI

	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-Incoming Materials	47.3	0	0.14	2.8E-04	0.14	6.1E-05	0.60	46.6	47.2
DNT/Phosgene/TDA/TDI Production	43.8	34.0	0	0.042	34.0	0	0	9.75	9.75
Total	**91.1**	**34.0**	**0.14**	**0.042**	**34.2**	**6.1E-05**	**0.60**	**56.3**	**56.9**
	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-Incoming Materials	47.3	0	0.14	2.8E-04	0.14	6.1E-05	0.60	46.6	47.2
DNT/Phosgene/TDA/TDI Production	43.8	34.0	0	0.042	34.0	0	0	9.75	9.75
Total	**91.1**	**34.0**	**0.14**	**0.042**	**34.2**	**6.1E-05**	**0.60**	**56.3**	**56.9**
	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-Incoming Materials	52%	0%	0.2%	0.00%	0.2%	0.00%	0.7%	51%	52%
DNT/Phosgene/TDA/TDI Production	48%	37%	0%	0.05%	37.4%	0%	0%	11%	11%
Total	**100%**	**37%**	**0.2%**	**0.05%**	**37.5%**	**0.00%**	**0.7%**	**61.8%**	**62.5%**

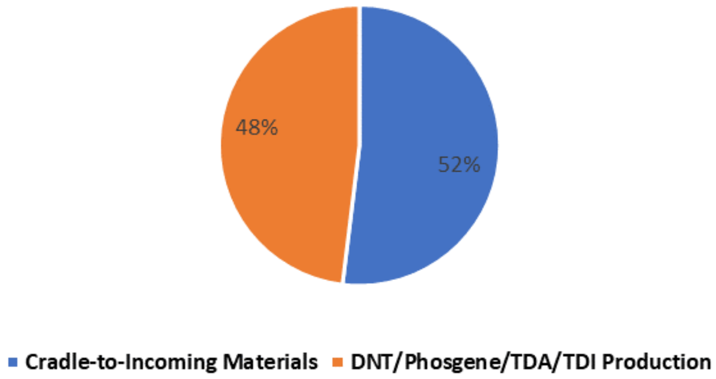

Figure 5. Percentage of Total Solid Wastes for TDI System

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. Water consumption attributed to hydropower generation does not include burdens for run of the river hydroelectric plants. Run-of-the-river facilities produce power with no artificial reservoir and thus exhibit no water consumption burden (Lampert, 2015).

Water consumption results for TDI production are shown in Table 5 and Figure 6. The greatest portion of consumption of water within the TDI comes from the cradle-to-incoming materials (92 percent). When looking at the individual input materials, 59 percent of the total is consumed by the cradle-to-gate manufacture of the chlorine and sodium hydroxide. The chlor-alkali process uses brine (saltwater solution) in the cell technology. The water consumption for toluene is 16 percent of the total for the system. Nitric acid and carbon monoxide production each make up between 9 and 14 percent of the water consumption total. The TDI plant water consumption makes up 8 percent of the total water consumed, which is split between electricity production (hydroelectric) and the production of natural gas for combustion at the plant.

Throughout all the unit processes, one of the larger contributors to water consumption is the electricity used, which makes up approximately 31 percent of the total water consumption. This is due to evaporative losses in the use of hydropower. Brine production and chlor-alkali cell technology also contribute 37 percent of the total water consumption; this amount does not include the water from the electricity required to power the cell. The extraction and processing of natural gas and oil used as a material and fuel comprise 15 percent of the total water consumption.

Table 5. Water Consumption for TDI

	Total Water Consumption		
	Basis: 1,000 Pounds	**Basis: 1,000 kilograms**	**Percentage of Total**
	Gallons	***Liters***	***%***
Cradle-to-Incoming Materials	695	5,802	92%
DNT/Phosgene/TDA/TDI Production	61	507	8%
Total	**756**	**6,309**	**100%**

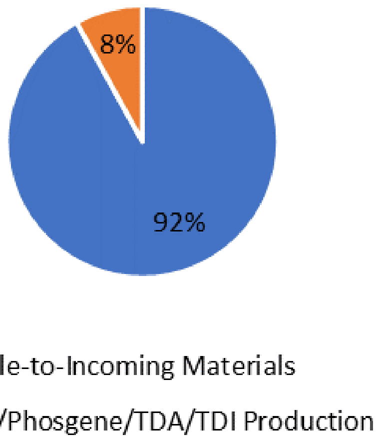

Figure 6. Water Consumption for TDI

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, methane, and nitrous oxide. Other contributors include some HCFCs and CFCs, but these contribute less than 1 percent of the total shown. Greenhouse gas emissions are mainly from combustion. In the primary data collected for chlor-alkali and TDI, combustion emissions from flare or another type of emissions control have been included as process emissions and so their totals may be overstated by small amounts due to the inclusion of combustion of fuel used during the use of the emissions control. Data providers were asked to estimate percentages of greenhouse gases from flares from that of the combustion of fuels.

The 100-year global warming potential (GWP) factors for each of these substances as reported in the Intergovernmental Panel on Climate Change (IPCC) 2013[18] 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.

In Table 6 and Figure 7, the life cycle GWP results for the TDI system are displayed. Of the total, 63 percent of the GWP are attributed to emissions from the incoming materials to the phosgene/DNT/TDA/TDI unit process, with the remaining associated with said unit process. Approximately 22 percent is created from the production of the carbon monoxide system, as well as 21 percent coming from the chlor-alkali system. The production of toluene and nitric acid systems together accounts for the remaining 20 percent of the total GWP.

Of the total GWP, 37 percent is associated with the phosgene/DNT/TDA/TDI unit process. Only 2 percent of the greenhouse gases for this unit process are released as a process emission at the plants; more than three-quarters of the remaining GWP for this unit process come from the combustion of natural gas in boilers on-site, while approximately 20 percent is created from the electricity grid or during off-site cogeneration electricity.

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[18] 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 TDI

	Global Warming Potential		
	Basis: 1,000 Pounds	Basis: 1,000 kilograms	Percentage of Total
	lb CO2 eq	*kg CO2 eq*	*%*
Cradle-to-Incoming Materials	1,298	1,298	63%
DNT/Phosgene/TDA/TDI Production	751	751	37%
Total	**2,049**	**2,049**	**100%**

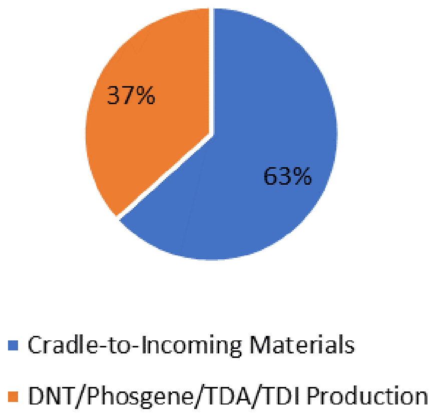

Figure 7. Global Warming Potential for TDI

Figure 8 displays the cradle-to-gate TDI GWP separated by process contribution. This figure illustrates the percentages of GWP specific to process emissions at individual unit processes (e.g., carbon monoxide production), as well as to fuel-related emissions from the combustion of fuels and fuel combustion for transportation. Only processes creating at least one percent of the total GWP have been shown individually; all processes contributing less than one percent have been grouped into "all other processes."

The largest amount of the GWP is created by the combustion of natural gas, coal, and oil in both industrial and utility boilers, which accounts for 56 percent of the total GWP. The production of carbon monoxide creates 17 percent of the GWP. Natural gas and oil extraction and processing/refining comprise 13 percent of the total GWP. Five percent of the total comes from the combustion of transport fuels including pipeline transport of natural gas and gas chemicals, which are two-thirds of that transport percentage. Toluene and nitric acid unit processes account for 4 and 3 percent of the GWP, respectively. All other processes are less than 1 percent individually and comprise 3 percent of the total GWP. The "all other processes" category includes the process greenhouse gases released at the TDI plants, which account for only 0.9 percent of the total; this is due to flaring or emission control processes, which is considered a mix of process and fuel-based emissions.

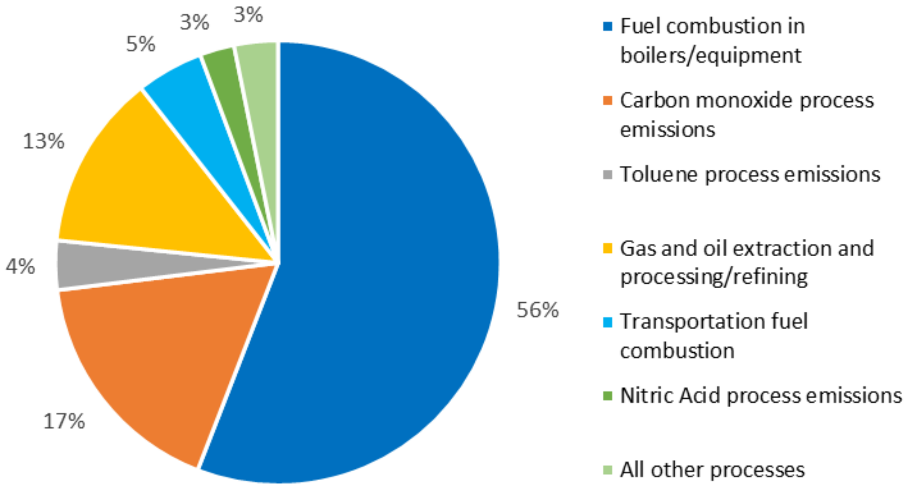

Figure 8. Global Warming Potential by Process Contribution

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 (AP) 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.[19,20]

Acidification impacts are typically dominated by fossil fuel combustion emissions, particularly sulfur dioxide (SO_2) and nitrogen oxides (NO_x). Emissions from combustion of coal to generate grid electricity is a significant contributor to acidification impacts for the system at 31 percent of the total AP. Combustion of natural gas comprise 9 percent of the total AP, which can be released on-site at plants or from electricity production. Also, emissions from the extraction and processing/refining of natural gas and oil impact the AP category at 37 percent of the total.

Table 7 shows total acidification potential results for the TDI system. Results are shown graphically in Figure 9. In the AP category, 25 percent of the AP is coming from TDI production and about 75 percent comes from the raw and intermediate material unit processes. Of the incoming materials AP, the greatest portion (29 percent of the total AP)

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[19] 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.

[20] 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.

comes from the chlor-alkali production which uses greater amounts of electricity. As stated previously, much of the acidification potential comes from the combustion of fuels in the industrial and utility boilers. The AP amounts for the nitric acid and toluene systems comprise 16 and 18 percent of the total AP respectively, with the remaining 12 percent from the carbon monoxide system.

Table 7. Acidification Potential for TDI

	Acidification Potential		
	Basis: 1,000 Pounds	Basis: 1,000 kilograms	Percentage of Total
	lb SO2 eq	*kg SO2 eq*	*%*
Cradle-to-Incoming Materials	3.68	3.68	75%
DNT/Phosgene/TDA/TDI Production	1.24	1.24	25%
Total	**4.91**	**4.91**	**100%**

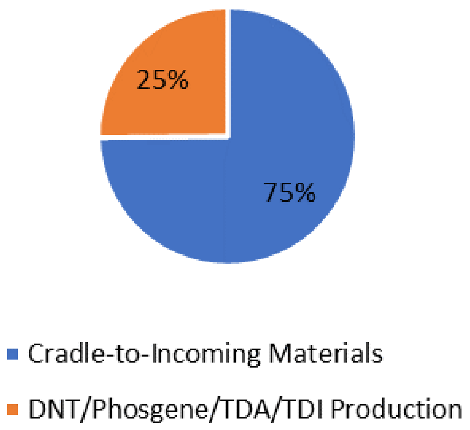

Figure 9. Acidification Potential for TDI

Looking specifically at the phosgene/DNT/TDA/TDI, which is 25 percent of the total AP, only 3 percent of the total AP comes directly from the associated process emissions of the TDI unit process. Over 15 percent of the AP shown in Table 7 for TDI production comes from the on-site industrial boilers using natural gas. Seven percent of the AP total is from the combustion of fuels used to create electricity for the phosgene/DNT/TDA/TDI processes.

EUTROPHICATION POTENTIAL

Eutrophication occurs when excess nutrients (nitrates, phosphates) are introduced to surface water causing the rapid growth of aquatic plants. Excess releases of these substances may provide undesired effects on the waterways.[21] The TRACI characterization factors for

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[21] 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.

eutrophication are the product of a nutrient factor and a transport factor.[22] 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 TDI are shown in Table 8 and illustrated in Figure 10. The largest portion, 69 percent, of the EP results come from the incoming materials to the phosgene/DNT/TDA/TDI production. The toluene system comprises the greatest EP amount of the incoming materials at 24 percent. Eight percent of the toluene EP is from process emissions from the toluene production, with the remaining from combustion of fuels and the extraction and processing of natural gas and oil. The cradle-to-nitric acid comprises almost 20 percent of the total EP amount, with 9 percent released during the nitric acid process, 8 percent released during the production of ammonia as an input to nitric acid, and the remaining from fuel combustion and natural gas and oil extraction and processing.

The emissions from the phosgene/DNT/TDA/TDI unit process comprise 31 percent of the total EP impact results. Almost 11 percent of the total EP impact comes from process emissions associated with the TDI plant. This is a combination of nitrogen oxides (likely flare or thermal oxidizer) and ammonia process emissions at the plant and waterborne releases of BOD and COD. Of the remaining, 17 percent represents the combustion of natural gas in boilers, with the remaining from utility boilers and a small amount from transport fuel combustion.

Table 8. Eutrophication Potential for TDI

	Eutrophication Potential		
	Basis: 1,000 Pounds	**Basis: 1,000 kilograms**	**Percentage of Total**
	lb N eq	***kg N eq***	***%***
Cradle-to-Incoming Materials	0.18	0.18	69%
DNT/Phosgene/TDA/TDI Production	0.080	0.080	31%
Total	**0.26**	**0.26**	**100%**

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[22] 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.

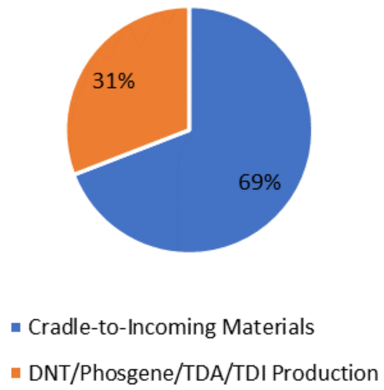

Figure 10. Eutrophication Potential for TDI

OZONE DEPLETION POTENTIAL

Stratospheric ozone depletion (ODP) is the reduction of the protective ozone within the stratosphere caused by emissions of ozone-depleting substances (e.g., CFCs and halons). The ozone depletion impact category characterizes the potential to destroy ozone based on a chemical's reactivity and lifetime. Effects related to ozone depletion can include skin cancer, cataracts, material damage, immune system suppression, crop damage, and other plant and animal effects. For the TDI system, the main sources of emissions contributing to ODP are minute amounts of tetrachloromethane, HCFCs, and halons emitted during the extraction of petroleum, which is used as fuel and material in the production of toluene.

Table 9 shows total ODP results for the TDI system, which are also shown graphically in Figure 11. The results of the ODP shown from TDI production makes up 99 percent and is mostly from HCFC-22, which is a refrigerant. Small leaks occur in refrigeration units infrequently according to producers. The collected data for this emission may be overstated as it was provided by only one producer of TDI and is representative of the original 2003 data. Ozone depletion results for the incoming materials to the TDI system are dominated by the crude oil extraction and refining used to create some of the incoming materials, contributing 1 percent of the total ozone depletion impacts.

Table 9. Ozone Depletion Potential for TDI

	Ozone Depletion Potential		
	Basis: 1,000 Pounds	Basis: 1,000 kilograms	Percentage of Total
	lb CFC-11 eq	*kg CFC-11 eq*	*%*
Cradle-to-Incoming Materials	2.7E-06	2.7E-06	1%
DNT/Phosgene/TDA/TDI Production	5.0E-04	5.0E-04	99%
Total	**5.0E-04**	**5.0E-04**	**100%**

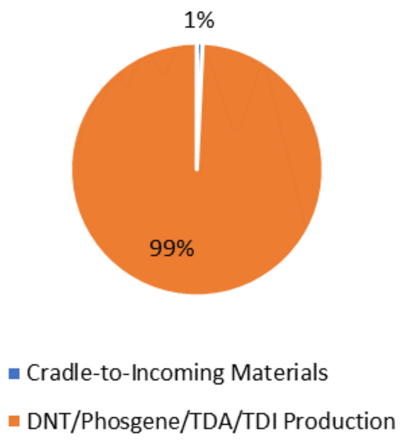

Figure 11. Ozone Depletion Potential for TDI

PHOTOCHEMICAL SMOG FORMATION

The photochemical ozone creation potential (POCP) impact category, also referred to as smog formation potential, 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.[23] 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 94 percent of the smog formation emissions, with VOCs consisting of over 5 percent.

Smog formation potential results for TDI are displayed in Table 10 and illustrated in Figure 12. Approximately 70% of the POCP impact results comes from the cradle-to-incoming materials. The toluene and chlor-alkali systems each produce approximately 21 percent of the total impact results in the POCP. The toluene system is assumed to be produced from petroleum, which creates two-thirds of the released emissions for that system. In the case of the chlor-alkali system, the POCP comes from the combustion of natural gas, coal, and other fuels for both industrial and utility boilers. The combustion and production of oil and gas also make up the largest POCP amounts for the other incoming materials.

The remaining 30 percent of the POCP impact results are released from the TDI production process. Of the total POCP for the TDI plant, 22 percent comes from the combustion of natural gas on-site. Less than 3 percent of the total emissions resulting in the POCP impact results are released at the TDI plant as process emissions. The remaining emissions from TDI production comes from the combustion of fuels to create electricity or transport the incoming materials.

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[23] 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.

Table 10. Photochemical Smog Formation Potential for TDI

	Photochemical Smog Potential		
	Basis: 1,000 Pounds	Basis: 1,000 kilograms	Percentage of Total
	lb O3 eq	***kg O3 eq***	***%***
Cradle-to-Incoming Materials	74.7	74.7	70%
DNT/Phosgene/TDA/TDI Production	31.4	31.4	30%
Total	**106**	**106**	**100%**

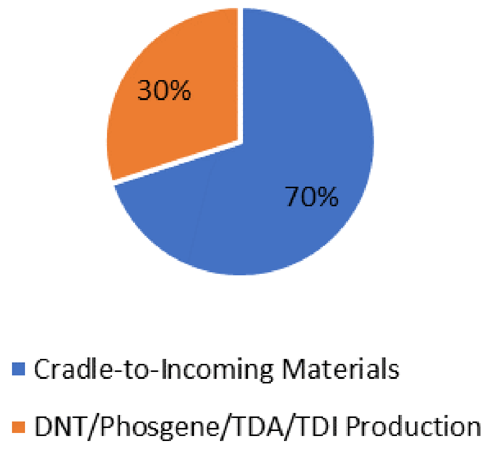

Figure 12. Photochemical Smog Formation Potential for TDI

COMPARISON OF 2022 AND 2011 LCI AND LCIA TDI RESULTS

This section provides a comparison of life cycle inventory and impact assessment category results that were included in the original cradle-to-gate TDI system[24] 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 2022 TDI results in both English and SI units and includes the percent change from the 2011 value for each category. Percent change between systems is defined as the difference between the 2022 and 2011 totals divided by the 2011 totals. The results in Table 11 show a decrease in energy and solid waste. There is a one percent increase in global warming potential. Comparisons of these results have been analyzed in this section focusing on the main differences causing the change in each category. It should be noted that all figures in this section provide a percent increase or decrease above the comparable bars.

It should be noted that the unit process for phosgene/DNT/TDA/TDI was not able to be updated as there were not three data providers in North America in 2016; however, data for incoming chemicals were updated as possible. Changes in results for the TDI plant are predominantly due to the change in electricity grid and change in method to using system expansion and avoided fuels. The update of incoming materials does include two updated primary datasets including the chlor-alkali and pygas (to create toluene) data. Each plant producing the chlor-alkali varies by the amounts of input materials used, fuel types and amounts used, amounts of emissions released, etc. The amalgamation of these changes lead to differences affecting the results for chlor-alkali average data. The chlor-alkali data represents the years 2015 (2 plants) and 2017 (1 plant). One chlor-alkali plant was included in the previous analysis, while the other two chlor-alkali data providers had not previously provided data and replaced data from chlor-alkali plant datasets from the 1990s, which improved the data quality of the analysis. The toluene data includes 70% from steam reforming from refined petroleum and 30% from pygas within the steam cracker; whereas the 2011 report used only the steam reforming process. Although the steam reforming data is older (circa 1990s) and originally from Europe, the data was adapted for the US and no major changes have occurred within the process itself. This adaptation likely decreased the energy and emissions for toluene due to changes in energy from use of oil products to natural gas. Finally, there was a decrease in energy and GWP for the natural gas and petroleum extraction and processing, which were updated from the 2011 original analysis.

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[24] 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 2022 LCI and LCIA Results for TDI

	1000 pounds of Toluene Diisocyanate				
	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***
TDI 2011	22.3	22.1	0.18	123	2,107
TDI 2022	19.8	19.7	0.13	91.1	2,049
	1000 kilograms of Toluene Diisocyanate				
	LCI Results				***LCIA Results***
	Total Energy	**Non-Renewable Energy**	**Renewable Energy**	**Total Solid Waste***	**Global Warming**
	GJ	***GJ***	***GJ***	***kg***	***kg CO_2 eq***
TDI 2011	51.8	51.4	0.43	123	2,107
TDI 2022	46.2	45.9	0.30	91.1	2,049
Percent Change	-11%	-11%	-30%	-26%	-3%

*Total Solid Waste includes hazardous solid waste for 2022 as this category was provided in the Solid Waste in 2011.

ENERGY COMPARISON

Overall, the total energy for the TDI system has decreased 5.6 GJ on a 1,000 kg basis (2.5 MMBtu/1,000 lb). There is an 11 percent decrease in total energy as compared to the original study's results. This percentage is due to differences mostly in the incoming materials, although the energy for the TDI plant did decrease as well. When comparing the phosgene/DNT/TDA/TDI unit process average total energy data from the original study and this 2022 update, there is a 5 percent decrease overall. The energy data itself did not change, so this difference is due to the change to the system expansion method to deal with the waste heat sent to other processes as well as the differences in the national average electricity grid. Figure 13 provides a graphical perspective of the unit processes associated with this energy decrease from the original energy amounts.

The energy of material resource, which pertains to the amount of inherent energy from the raw materials increased by 5 percent for TDI due to the changes in the amount of raw material inputs from data updates compared to the data in the 2011 report. As the amount of material resource energy increased, but the total energy still decreased, it can be concluded that the difference in process energy decreased by a slightly greater percentage than the 11 percent shown in the total. Besides the decrease in TDI production, this decrease is also due to the energy decreases in the energy requirements for the oil and natural gas extraction and processing/refining, which are used to produce the carbon monoxide, ammonia (input to nitric acid), and toluene.

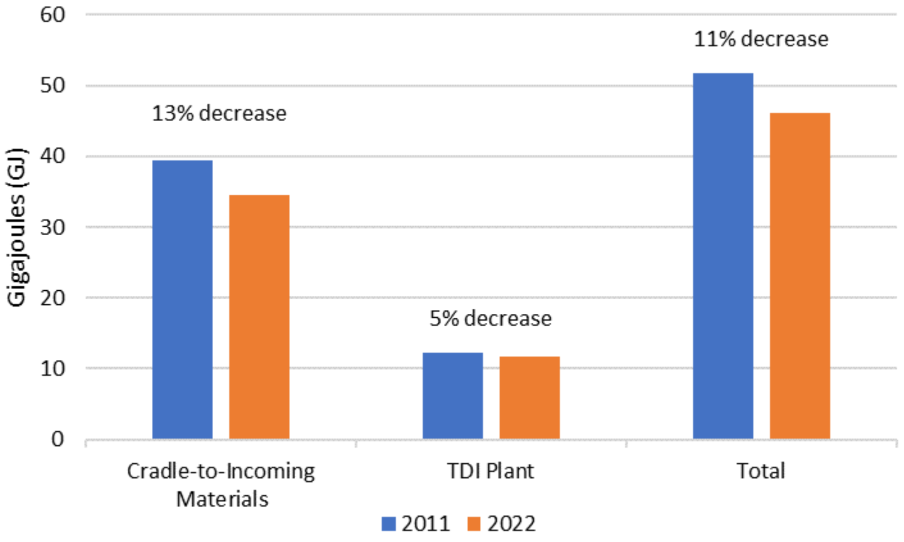

Figure 13. Change in Energy by Stage per 1,000 kg (GJ)

SOLID WASTE COMPARISON

When compared to the 2011 TDI total solid waste amount, the current TDI analysis shows 31.9 kg per 1000 kg less solid waste, which is a 26 percent decrease from the original study. Figure 14 provides a visual of the total solid waste amount split out by the TDI unit process and cradle-to-incoming materials. Most of this decrease is due to the differences in the cradle-to-intermediate chemicals data between the 2011 and 2022 reports; however, there is a 10 percent decrease in the phosgene/DNT/TDA/TDI solid waste data. As no new data was collected this decrease is due to changes in the electricity grid, likely the decrease in coal use and increase in natural gas use in the grid. A decrease also occurs for cradle-to-incoming materials. The decrease in cradle-to-incoming materials is due to differences in the datasets used, lower amounts of solid waste at the chlor-alkali plants, as well as the change in the electricity grid fuels for all processes. Process solid wastes from the natural gas and crude oil production also decreased by small amounts.

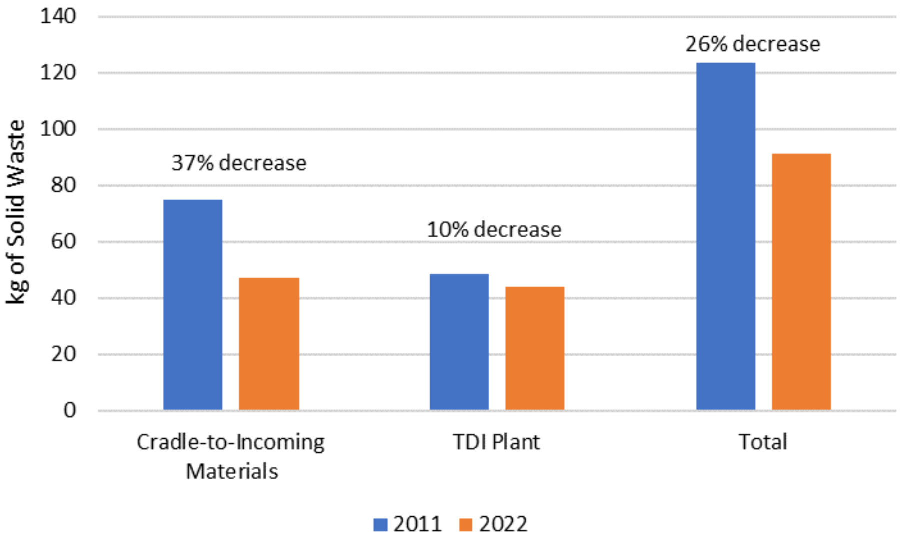

Figure 14. Change in Solid Waste Weight by Unit Process (kg Per 1,000 kg)

GLOBAL WARMING POTENTIAL COMPARISON

The total global warming potential decreased by 58 kg CO2 equivalents/1000 kg of TDI, which calculates to a 3 percent decrease. Figure 15 displays a column chart with the TDI and cradle-to-incoming materials results that makeup the decrease when comparing the 2011 and 2022 GWP results. Although the overall GWP decreased, a very small increase is seen in the incoming materials to the TDI unit process. The total energy amount includes the material resource energy, which has no greenhouse gases associated with it as it is not combusted. The material resource energy did increase by a small amount while the overall energy decreased. Much of the greenhouse gases are created from fuel production.

The GWP specific to the TDI plant decreased by 8 percent, while the energy for the plant also decreased by close to that same percentage. This is due to the change in fuel mix of the electricity grid, as well as the change to system expansion methodology for waste heat. Previously, only an energy credit was given to the waste heat, but in the system expansion method, credit is also given to the emissions that are not released due to the use of the waste heat instead. The small increase in GWP for the cradle-to-incoming materials is a mix of changes to the electricity grid fuels, differences in datasets used, and updates to primary data for chlor-alkali inputs. The amount of coal combusted for the US average electricity grid has decreased over time with an increase in natural gas combustion. Coal production and combustion releases higher amounts of greenhouse gases compared to natural gas production and combustion. The GWP for some input materials increased while others decreased. The increase was driven largely by the carbon monoxide system GWP increase, while the toluene system GWP decreased due to changes in the dataset.

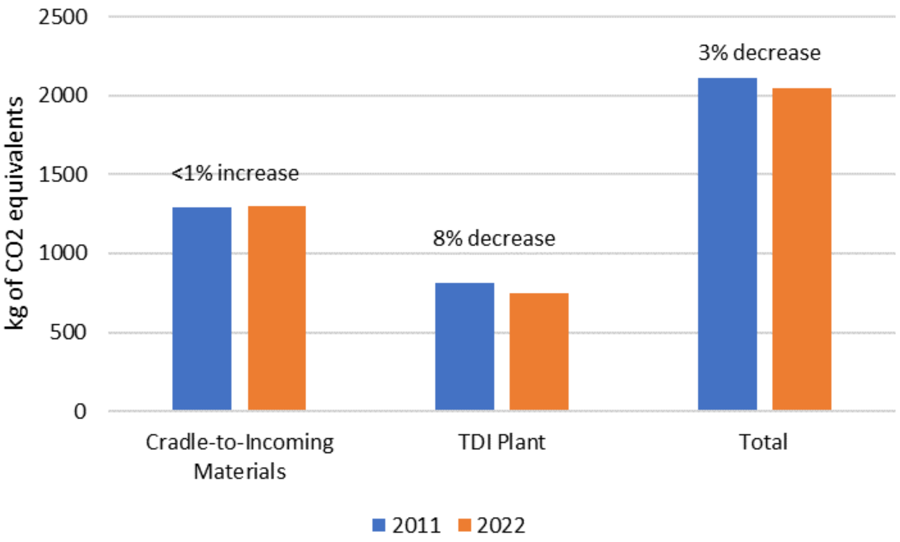

Figure 15. Change in Global Warming Potential by Unit Process (kg of CO2 eq. per 1,000 kg)

It should also be noted that the characterization factors for the GWP have changed since the 2011 report. The methane amount increased from 25 to 28 lb CO2eq/1 lb methane and the nitrous oxide amount decreased from 298 to 265 lb CO2eq/1 lb. As the methane and nitrous oxide releases account for less than 5 percent of the GWP characterization, the change in results due to this characterization factor difference is small but may be meaningful due to the small changes shown in the total.

SENSITIVITY ANALYSIS

For this TDI report, results using mass allocation for TDI/HCl are provided in the results section. Recently, the European Diisocyanate and Polyol Producers Association (ISOPA) released a new dataset for TDI and TDI for European manufacturers that uses a combined elemental and mass allocation.[25] This sensitivity analysis is included to provide results for both allocation methods as was done in the ISOPA study. The results using a mass allocation allow the reader to compare to the original 2011 TDI results; while the results using combined elemental + mass allocation allow the reader to compare the current North American TDI results to the current EU TDI results. Also provided are results using the TDI datasets from the original 2011 report using the elemental + mass allocation as a comparison. It should be noted that the TDI plant data is equivalent for the 2011 and 2022 analysis. The differences lie in the incoming material datasets, the electricity grid fuel differences and use of system expansion method.

Table 12 provides the results on a 1,000 kg basis using both mass and the elemental + mass allocation methods for both the 2011 LCI data as well as the 2022 LCI data. When comparing the results of the two allocation methods for either year, an increase is seen when using the elemental + mass allocation. The mass of hydrochloric acid created from the process of creating TDI is almost one third of the output by weight. When mass allocation is used, almost a third of the resulting impacts are given to the HCl, which is why there is a substantial decrease in the results when this allocation method is used. When the inputs to DNT and Phosgene are allocated to the TDI alone as done in the elemental + mass allocation, most of the resulting impacts increase. The exceptions are renewable energy and water consumption, these are due to the removal of chlorine production. The chlor-alkali process uses mainly electricity, which is where the renewable energy sources are from, plus uses water within the brine input to the process. The solid waste also increases by a small amount for the 2011 data. In this case, the process emissions increased with the change in method, but the fuel emissions decreased (due to the allocation of chlorine to HCl) by almost the same amount.

Focusing on the 2022 total energy for both allocation methods, there is an increase of 51 percent when switching to the elemental + mass allocation method. The 2011 change in allocation method shows a similar increase. The global warming potential calculated for 2022 increases by 36 percent if the elemental + mass allocation is used. Although much of the GWP is based on the energy amount, the smaller increase is due to the inclusion of feedstock energy in the energy shown, which would all be allocated to the TDI and would carry no GWP amount as is inherent in the plastic and not combusted. The 2011 GWP increase is less, this is likely due to the differences in the data sources & chlorine primary data update.

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[25] ISOPA Eco-profile of toluene diisocyanate (TDI) and methylene diphenyl diisocyanate (TDI). April 2021.

Table 12. Comparison of 2011 and 2022 LCI and LCIA Results for 1,000 kg of TDI Using Both Mass and Elemental + Mass Allocation Methods

	1,000 kilogram of TDI									
	LCI Results					*LCIA Results*				
	Total Energy	**Non-Renewable Energy**	**Renewable Energy**	**Water Consumption**	**Total Solid Waste**	**Global Warming**	**Acidification**	**Eutrophication**	**Ozone Depletion**	**Smog Formation**
	GJ	***GJ***	***GJ***	***Liters***	***kg***	***kg CO2 eq***	***kg SO2 eq***	***kg N eq***	***kg CFC-11 eq***	***kg O3 eq***
NA TDI **2011** (Mass allocation)	51.8	51.4	0.43	NA	123	2.11	NA	NA	NA	NA
NA TDI **2011** (Elemental+Mass allocation)	77.9	77.5	0.32	NA	121	2.60	NA	NA	NA	NA
NA TDI **2022** (Mass allocation)	46.2	45.9	0.30	6,309	91.1	2.05	4.91	0.26	5.0E-04	106
NA TDI **2022** (Elemental+Mass allocation)	69.9	69.7	0.19	4,791	97.2	2.79	6.18	0.39	5.0E-04	148

APPENDIX: TOLUENE DIISOCYANATE (TDI) MANUFACTURE

This appendix discusses the manufacture of TDI, which is a precursor in the manufacture of primarily flexible polyurethane foams that are used for carpet pads, furniture cushions, construction, insulation, and packaging. The unit process for TDI includes the manufacture of both pure and polymeric TDI. Due to the confidentiality of some datasets, phosgene and DNT are aggregated with TDA/TDI. The flow diagram of processes included for phosgene/DNT/TDA/TDI is provided in Figure 16.

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 discussed in this appendix:

- Toluene
- Phosgene
- Dinitrotoluene (DNT)
- Toluene diamine (TDA)
- Toluene diisocyanate (TDI)

Primary LCI data for chlorine and sodium hydroxide were collected for this update to the U.S. LCI plastics database by both member and non-member companies of the American Chemistry Council. No updated primary data was used for the phosgene/DNT/TDA/TDI unit process; however, the primary data collected from the year 2003 was used with the 2016 electricity grid and the system expansion method for waste gas sent to other processes. Secondary LCI data was used for ammonia, nitric acid, carbon monoxide, crude oil extraction and refining and natural gas production and processing. LCI data for the production of crude oil and natural gas and pygas production can be found in the report, ***Cradle-to-Gate Life Cycle Analysis of Olefins*** (Franklin Associates, 2020). LCI data for the production of sodium chloride (salt) solution mining, chlor-alkali (chlorine and sodium hydroxide) are presented in the report, ***Cradle-to-Gate Life Cycle Analysis of Polyvinyl Chloride (PVC) Resin*** (Franklin Associates, 2021). LCI data for salt mining was adapted from the ecoinvent 3 database. The adaptations included the use of the US electricity grid and US transportation. LCI data for the production of ammonia, carbon monoxide and nitric acid, are found in the report, ***Cradle-to-Gate Life Cycle Analysis of Methylene diphenyl diisocyanate (MDI)*** (Franklin Associates, 2022).

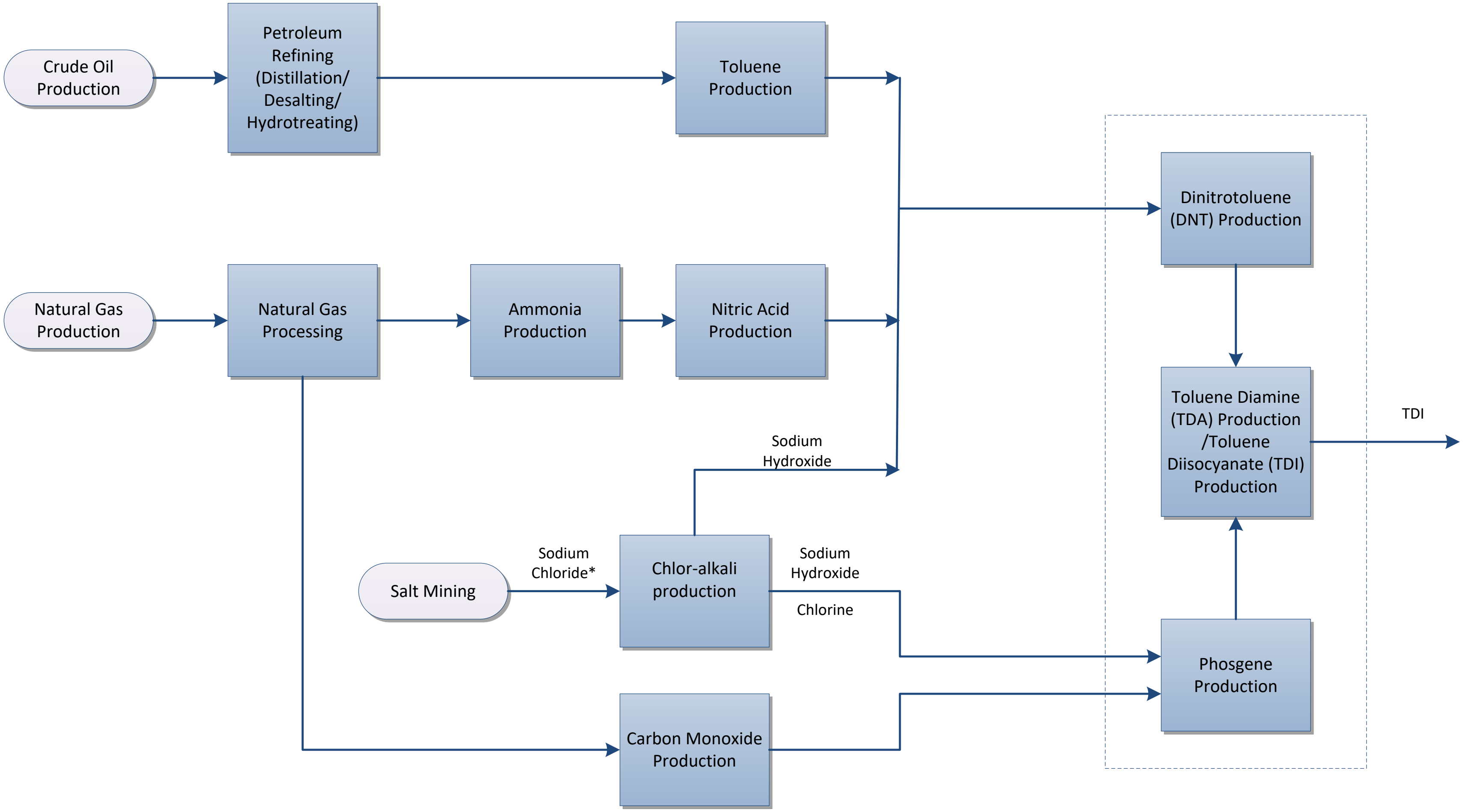

Figure 16. Flow diagram for the Production of Toluene Diisocyanate (TDI).
* Sodium chloride data are from ecoinvent and are adapted to U.S. conditions.

Toluene Production

Approximately 70 percent of global toluene is produced by the catalytic reforming of light petroleum distillate (naphtha) (Egun, 2018). Toluene can also be produced from pyrolysis gas or as a coproduct of styrene from ethylbenzene. Available data for toluene from the catalytic reforming of naphtha comes from Europe in the 1990s and has been adapted to the US for this analysis as 70 percent of the dataset. The remaining 30 percent uses the primary production of pyrolysis gas. Data for the BTX separation stage is not included in the pyrolysis gas percentage of the dataset.

In the reforming process, naphtha is fed through a series of three catalyst bed reactors at elevated temperatures and pressures. A common catalyst used in reforming reactions includes a platinum/rhenium/aluminum oxide catalyst (0.3 wt% Pt, 0.3 wt% Re)(Meidanshahi et al., 2011). Reformate products obtained from the process include aromatic compounds (benzene, toluene, xylene) and high-octane gas reformate. The aromatics content of the reformate varies and is normally less than 45 percent. The reformate from conventional naphtha process undergoes solvent extraction and fractional distillation to produce pure benzene, toluene, and other coproducts.

The energy requirements and environmental emissions for the production of toluene are shown in Table 13. This table includes a split of 70% steam reforming data and 30% pygas data. The catalytic reforming portion of this data are calculated from a straight average of two catalytic reformer datasets from Europe in the early 1990s. These data were reviewed and adapted for US conditions. Overall, the catalytic reforming process has not undergone major changes over the past 30 years. Updated LCI data for the production of toluene from catalytic reforming was not found for this analysis. The pyrolysis gas dataset comes from the 2018 ACC olefins report. The pyrolysis gas dataset does not include the separation of the benzene/toluene/xylenes streams.

Table 13. LCI Data for the Production of Toluene

	1,000 lb	1,000 kg
Material Inputs (1)		
Refined Petroleum Products	733 lb	733 kg
Processesed Natural Gas	267 lb	267 kg
Internal off-gas (2)		
From oil	6.30 lb	6.30 kg
From natural gas	48.0 lb	48.0 kg
Energy		
Process Energy		
Electricity from grid	10.5 kWh	23.2 kWh
Electricity from cogen	3.42 kWh	7.53 kWh
Natural gas	1,101 ft^3	68.7 m^3
Fuel Gas	603 ft^3	37.6 m^3
Landfill gas	2.45 ft^3	0.15 m^3
Avoided Energy		
Oil sold as co-product	0.11 gal	0.0010 m^3
Recovered energy from exported steam	77.8 ft^3	4.85 m^3
Off-gas sold	177 ft^3	11.0 m^3
Transportation Energy		
Barge	8.42 ton·mi	27.1 tonne·km
Pipeline -refinery products	9.06 ton·mi	29.2 tonne·km
Pipeline -natural gas products	76.7 ton·mi	247 tonne·km

Phosgene Production

Phosgene (also called carbonyl chloride, carbon oxychloride, or chloroformyl chloride) is produced by the reaction of carbon monoxide and chlorine in the presence of an activated charcoal catalyst. Careful production, handling, and trace recovery must be maintained because of phosgene's toxicity. Chlorine gas and carefully purified carbon monoxide are mixed with a slight excess of carbon monoxide to insure complete conversion of chlorine. The reaction is exothermic and is carried out in relatively simple tubular heat exchangers. (Rossi et al., 2021) The product gas is condensed, and the phosgene removed in an absorption column. Any non-condensed phosgene is removed in a caustic scrubber.

Phosgene data collected on-site as part of the same plant producing TDI for 2003 and is included in Table 16 and Table 17.

Table 14. LCI Data for the Production of Toluene (continued)

	1,000 lb	1,000 kg	
Environmental Emissions			
Atmospheric Emissions			
Particulates, unspecified	0.017 lb	0.017 kg	*
Particulates, < 2.5 um	0.0075 lb	0.0075 kg	
Particulates, > 2.5 um, and < 10um	0.0014 lb	0.0014 kg	
Nitrogen oxides	0.13 lb	0.13 kg	
NMVOC, non-methane volatile organic compounds, u	0.037 lb	0.037 kg	
VOC, volatile organic compounds	0.0030 lb	0.0030 kg	*
Sulfur oxides	0.31 lb	0.31 kg	
Carbon dioxide, fossil	221 lb	221 kg	
Methane, fossil	0.031 lb	0.031 kg	
Nitrous oxide	0.066 lb	0.066 kg	
Carbon monoxide	0.082 lb	0.082 kg	
Hydrogen sulfide	3.0E-07 lb	3.0E-07 kg	*
Ammonia	3.0E-04 lb	3.0E-04 kg	*
Chlorine	3.0E-06 lb	3.0E-06 kg	*
Waterborne Releases			
Benzene	0.0030 lb	0.0030 kg	*
BOD5, Biological Oxygen Demand	0.49 lb	0.49 kg	
COD, Chemical Oxygen Demand	0.89 lb	0.89 kg	
Benzene, ethyl-	3.0E-04 lb	3.0E-04 kg	*
Phenol	3.0E-05 lb	3.0E-05 kg	*
Styrene	0.0030 lb	0.0030 kg	*
Suspended solids, unspecified	0.080 lb	0.080 kg	*
Toluene	0.0030 lb	0.0030 kg	*
TOC, Total Organic Carbon	3.0E-07 lb	3.0E-07 kg	*
Xylene	3.0E-04 lb	3.0E-04 kg	*
Dissolved solids	3.0E-06 lb	3.0E-06 kg	*
Cyanide	3.0E-07 lb	3.0E-07 kg	*
Nickel	3.0E-07 lb	3.0E-07 kg	*
Mercury	3.0E-08 lb	3.0E-08 kg	*
Lead	3.0E-08 lb	3.0E-08 kg	*
Ammonia	3.0E-04 lb	3.0E-04 kg	*
Ethylene glycol	3.0E-04 lb	3.0E-04 kg	*
Propylene glycol	3.0E-04 lb	3.0E-04 kg	*
Ethene	0.0030 lb	0.0030 kg	*
Butadiene	3.0E-04 lb	3.0E-04 kg	*
Isoprene	3.0E-05 lb	3.0E-05 kg	*
Cresol	3.0E-06 lb	3.0E-06 kg	*
Biphenyl	3.0E-04 lb	3.0E-04 kg	*
7,12-Dimethylbenz(a)anthracene	3.0E-06 lb	3.0E-06 kg	*
3-Methylcholanthrene	3.0E-07 lb	3.0E-07 kg	*
Sodium Bisulfate	3.0E-06 lb	3.0E-06 kg	*
Dimethyl phthalate	3.0E-05 lb	3.0E-05 kg	*
Dibenz(a,j)acridine	3.0E-07 lb	3.0E-07 kg	*
Oil, unspecified	0.013 lb	0.013 kg	
Sulfides	7.0E-04 lb	7.0E-04 kg	

Table 15. LCI Data for the Production of Toluene (continued)

	1,000 lb		1,000 kg	
Solid Wastes				
Solid waste, process to landfill	0.11	lb	0.11	kg
Solid waste, process to incineration	1.95	lb	1.95	kg
Solid waste, process to waste-to-energy incineration	2.0E-04	lb	2.0E-04	kg
Solid Waste Sold for Recycling or Reuse	0.063	lb	0.063	kg
Hazardous waste to landfill	9.0E-04	lb	9.0E-04	kg
Hazardous waste to incineration	0.45	lb	0.45	kg
Water Consumption	121	gal	1.01	m^3

* For the pygas portion of this dataset, 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

References: Primary data 1990, Franklin, 2020, and Franklin 2022a

Dinitrotoluene (DNT) Production

Nitroaromatics, including nitrobenzene, nitrochlorobenzene, and dinitrotoluene, are formed by nitrating the appropriate aromatic hydrocarbon with a mixed acid containing nitric and sulfuric acid. In the first stage of the nitration process a mixture of the ortho-, meta-, and para-nitrotoluene isomers is formed. The ortho- and para-nitrotoluene isomers are separated from the acid mixture in a centrifugal separator. After the isomers are separated, they are reacted with nitric acid to produce either 2,4-DNT or a mixture of 2,4-DNT and 2,6-DNT. The recovered acid mixture containing excess nitric acid, dissolved organics and gaseous nitric oxide is recycled (Chem, 2022).

Sulfuric acid is separated and recycled back into the production of nitroaromatics. Since sulfuric acid does not leave the process as part of the product, it is treated as a catalyst. Only the make-up sulfuric acid is included in the LCI.

Data for the production of DNT was collected from one confidential source for 2003 in the United States. To ensure confidentiality, this data was aggregated with phosgene, TDA, and TDI and is included in Table 16 and Table 17.

Toluene diamine (TDA) Production

Toluene Diamine (TDA) is produced by the hydrogenation of dinitrotoluene in a continuous stirred tank reactor. The catalytic hydrogenation of dinitrotoluene to toluene diamine is a standard aromatic synthesis process that produces a TDA-water mixture. The isomer ratio for TDA depends on the DNT isomer ratio used. Water and ortho-TDA can be removed by distillation and ortho TDA is sold or recycled, leaving meta TDA. The meta TDA stream includes an 80:20 mixture of 2,4- and 2,6-TDA.(Chem, 2022).

Because confidential datasets cannot be shown individually, the datasets for phosgene, DNT, TDA, and TDI were aggregated into one dataset. TDA data was collected from two sources and are included with the TDI energy and emissions in Table 16 and Table 17. The TDA producers verified that the characteristics of their plants are representative of a majority of North American TDA production. The average phosgene/DNT/TDA/TDI dataset was reviewed and accepted by all phosgene/DNT/TDA/TDI data providers. The data submitted for TDA represents U.S. production in the year 2003.

Toluene Diisocyanate (TDI) Production

Toluene diisocyanate (TDI) is made by phosgenation of toluene diamine (TDA). The diamine mixture is dissolved in chlorobenzenes and reacts with excess phosgene to produce the TDI. After phosgenation, the mixture is stripped from the solvent and separated by distillation (Chem, 2022). The excess phosgene is recycled. Most of the TDI used in flexible polyurethane foams is a mixture of the 2,4- and 2,6- isomers. The 80:20 mixture of 2,4-TDI and 2,6-TDI is the most important commercial product, but other mixtures are available (Korbaks et al., 2018).

Tables 14 and 15 presents the data for the production of TDI aggregated with phosgene, DNT and TDA. Data for the production TDI were provided by three leading producers (3 plants) for 2003 in North America. Waste heat was exported as a coproduct for some producers. System expansion was used to give credit to the use of natural gas that was avoided by using the waste heat. In 2015, there were only 2 companies manufacturing TDI in North America; therefore, it was decided that the 2003 average data would be used after comparing the data to current data provided by one manufacturer. Differences in data were minor overall, with lower energy consumption the main difference.

Table 16 presents the LCI data for the production of phosgene, DNT, TDA, and PTDI/TDI with a mass allocation for the products TDI and HCl, while Table 17 presents the LCI data using the elemental + mass allocation. The unit process using both allocation methods have been provided here although only results for mass allocation are shown in the body of the report. The elemental + mass allocation results have been shown in a sensitivity analysis.

A large amount of hydrogen chloride is produced as a coproduct during this process. As stated previously, a mass basis was used to partition the credit for each product in the main results of the study. Once collected, the data for each plant is reviewed individually. At that time, coproduct allocation is performed for the individual plant. After coproduct allocation is complete, the data of all plants are averaged using yearly production amounts. This was also done using the elemental + mass allocation method for each plant with results using this allocation shown in the Sensitivity Analysis section.

Table 16. LCI Data for the Production of Toluene Diisocyanate (TDI) – Mass Allocation

	1,000 lb		1,000 kg		
Material Inputs					
Carbon monoxide	192	lb	192	kg	
Toluene	308	lb	308	kg	
Chlorine	462	lb	462	kg	
Sodium Hydroxide	22.6	lb	22.6	kg	
Nitric acid	431	lb	431	kg	
Energy					
Process Energy					
Electricity from grid	29.5	kWh	65.0	kWh	
Electricity from cogen	116	kWh	256	kWh	
Natural gas	3,992	ft^3	249	m^3	
Avoided Energy (1)					
Natural gas avoided	327	ft^3	20	m^3	
Transportation Energy					
Barge	2.30	ton·mi	7.40	tonne·km	
Pipeline - petroleum products	0.21	ton·mi	0.69	tonne·km	
Pipeline - gas products	0.90	ton·mi	2.90	tonne·km	
Truck	0.068	ton·mi	0.22	tonne·km	
Rail	3.98	ton·mi	12.8	tonne·km	
Environmental Emissions					
Atmospheric Emissions					
Ammonia	0.049	lb	0.049	kg	
Benzene, 1,2-dichloro-	0.0010	lb	0.0010	kg	*
Carbon monoxide	0.010	lb	0.010	kg	*
Phosgene	1.0E-05	lb	1.0E-05	kg	*
Chlorine	2.8E-04	lb	2.8E-04	kg	
Methane, chlorodifluoro-, HCFC-22	0.015	lb	0.015	kg	
NMVOC, non-methane volatile organic compounds, u	0.024	lb	0.024	kg	
Hydrogen chloride	0.0010	lb	0.0010	kg	*
Lead	1.0E-07	lb	1.0E-07	kg	*
Mercury	1.0E-07	lb	1.0E-07	kg	*
Nitrogen oxides	0.12	lb	0.12	kg	
Organic substances, unspecified	1.0E-04	lb	1.0E-04	kg	*
Particulates, unspecified	0.0057	lb	0.0057	kg	
Particulates, < 2.5 um	0.0010	lb	0.0010	kg	*
Particulates, > 2.5 um, and < 10um	0.011	lb	0.011	kg	
Toluene, 2,4-diamine	1.0E-05	lb	1.0E-05	kg	*
Toluene diisocyanate	1.0E-04	lb	1.0E-04	kg	*

Table 14. LCI Data for the Production of Toluene Diisocyanate (TDI) – Mass Allocation (continued)

	1,000 lb	**1,000 kg**	
Waterborne Releases			
Ammonia	1.0E-04 lb	1.0E-04 kg	*
Benzene, 1,2-dichloro-	1.0E-04 lb	1.0E-04 kg	*
BOD5, Biological Oxygen Demand	0.050 lb	0.050 kg	
Chloroform	1.0E-06 lb	1.0E-06 kg	*
COD, Chemical Oxygen Demand	0.17 lb	0.17 kg	
Copper	1.0E-06 lb	1.0E-06 kg	*
Cyanide	3.0E-05 lb	3.0E-05 kg	
Dissolved solids	1.00 lb	1.00 kg	*
Nickel	1.0E-06 lb	1.0E-06 kg	*
Nitrate compounds	0.010 lb	0.010 kg	*
Phosphate	0.0010 lb	0.0010 kg	*
Sodium hydroxide	1.00 lb	1.00 kg	*
Suspended solids, unspecified	0.037 lb	0.037 kg	
TOC, Total Organic Carbon	0.010 lb	0.010 kg	*
Solid Wastes			
Solid waste, process to landfill	0.10 lb	0.10 kg	
Hazardous waste to landfill	0.042 lb	0.042 kg	
Hazardous waste to WTE	34.0 lb	34.0 kg	

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(1) Avoided energy is heat is produced during the process. This has been included as natural gas using system expansion.

* 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.

References: Primary data 2003

Table 17. LCI Data for the Production of Toluene Diisocyanate (TDI) – Elemental + Hybrid Allocation

	1,000 lb		1,000 kg		
Material Inputs					
Carbon monoxide	363	lb	363	kg	
Toluene	584	lb	584	kg	
Sodium Hydroxide	26.8	lb	26.8	kg	
Nitric acid	815	lb	815	kg	
Energy					
Process Energy					
Electricity from grid	34.1	kWh	75.2	kWh	
Electricity from cogen	145	kWh	320	kWh	
Natural gas	6,281	ft^3	392	m^3	
Avoided Energy (1)					
Natural gas avoided	327	ft^3	20.4	m^3	
Transportation Energy					
Barge	4.35	ton·mi	14.0	tonne·km	
Pipeline - petroleum products	0.40	ton·mi	1.30	tonne·km	
Pipeline - gas products	1.24	ton·mi	3.98	tonne·km	
Truck	0.12	ton·mi	0.40	tonne·km	
Rail	7.77	ton·mi	25.0	tonne·km	
Environmental Emissions					
Atmospheric Emissions					
Ammonia	0.078	lb	0.078	kg	
Benzene, 1,2-dichloro-	0.0010	lb	0.0010	kg	*
Carbon monoxide	0.010	lb	0.010	kg	*
Phosgene	1.0E-05	lb	1.0E-05	kg	*
Methane, chlorodifluoro-, HCFC-22	0.010	lb	0.010	kg	*
NMVOC, non-methane volatile organic compounds, u	0.024	lb	0.024	kg	
Lead	1.0E-07	lb	1.0E-07	kg	*
Mercury	1.0E-07	lb	1.0E-07	kg	*
Nitrogen oxides	0.14	lb	0.14	kg	
Organic substances, unspecified	1.0E-04	lb	1.0E-04	kg	*
Particulates, < 2.5 um	0.0010	lb	0.0010	kg	*
Particulates, > 2.5 um, and < 10um	0.011	lb	0.011	kg	
Toluene, 2,4-diamine	1.0E-05	lb	1.0E-05	kg	*
Toluene diisocyanate	1.0E-04	lb	1.0E-04	kg	*

Table 15. LCI Data for the Production of Toluene Diisocyanate (TDI) – Elemental + Hybrid Allocation (continued)

	1,000 lb	1,000 kg	
Waterborne Releases			
Ammonia	1.0E-04 lb	1.0E-04 kg	*
Benzene, 1,2-dichloro-	1.0E-04 lb	1.0E-04 kg	*
BOD5, Biological Oxygen Demand	0.093 lb	0.093 kg	
Chloroform	1.0E-06 lb	1.0E-06 kg	*
COD, Chemical Oxygen Demand	0.32 lb	0.32 kg	
Copper	1.0E-06 lb	1.0E-06 kg	*
Cyanide	5.6E-05 lb	5.6E-05 kg	
Dissolved solids	1.00 lb	1.00 kg	*
Nickel	1.0E-06 lb	1.0E-06 kg	*
Nitrate compounds	0.010 lb	0.010 kg	*
Phosphate	0.0010 lb	0.0010 kg	*
Sodium hydroxide	1.00 lb	1.00 kg	*
Suspended solids, unspecified	0.037 lb	0.037 kg	
TOC, Total Organic Carbon	0.010 lb	0.010 kg	*
Solid Wastes			
Solid waste, process to landfill	0.10 lb	0.10 kg	
Hazardous waste to landfill	0.042 lb	0.042 kg	
Hazardous waste to WTE	34.0 lb	34.0 kg	

(1) Avoided energy is heat is produced during the process. This has been included as natural gas using system expansion.

* 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.

References: Primary data, 2003.

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