REVISED FINAL APPENDICES

CRADLE-TO-GATE LIFE CYCLE INVENTORY OF NINE PLASTIC RESINS AND FOUR POLYURETHANE PRECURSORS

Prepared for

PLASTICS DIVISION OF THE AMERICAN CHEMISTRY COUNCIL (ACC)

by

FRANKLIN ASSOCIATES,
A DIVISION OF EASTERN RESEARCH GROUP, INC.
Prairie Village, Kansas

August, 2011

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APPENDIX A

ENERGY REQUIREMENTS AND ENVIRONMENTAL EMISSIONS FOR FUEL CONSUMPTION

Franklin Associates is updating our Fuels Appendix at this time. This Appendix will be completed and available within this document by August 31, 2011.

APPENDIX B

HIGH-DENSITY POLYETHYLENE

INTRODUCTION

This appendix discusses the manufacture of high-density polyethylene (HDPE) resin. Large amounts of HDPE resin are used to manufacture blow-molded bottles, piping, film, and pails. Almost 16 billion pounds of HDPE was produced in the U.S. and Canada in 2003 (Reference B-1). The material flow for HDPE resin is shown in Figure B-1. The total unit process energy and emissions data (cradle-to-HDPE) for HDPE are displayed in Table B-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. The following processes are included in this appendix:

- Crude oil production
- Distillation, desalting, and hydrotreating
- Natural gas production
- Natural gas processing
- Olefins (Ethylene) production
- HDPE resin production

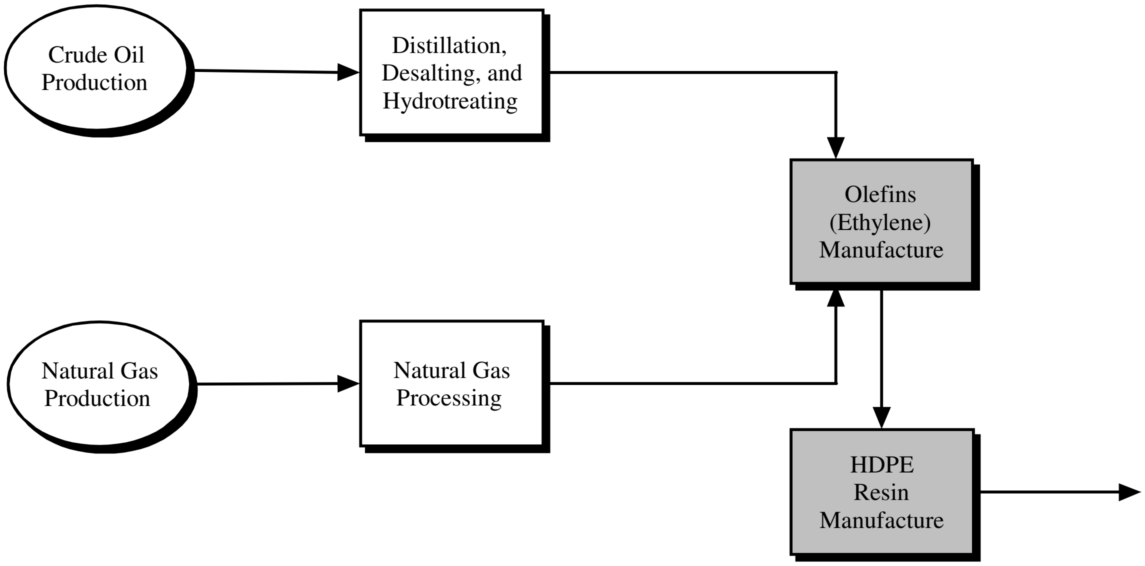


Figure B-1. Flow diagram for the manufacture of virgin high-density polyethylene (HDPE) resin. Shaded boxes represent partial or complete data provided by manufacturers specifically for this APC analysis.

Table B-1

DATA FOR THE PRODUCTION
OF HIGH-DENSITY POLYETHYLENE (HDPE) RESIN
(Cradle-to-Resin)
(page 1 of 3)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	188	lb		188	kg	
Natural Gas	827	lb		827	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			17,701			41.2
Petroleum			3,520			8.20
Total Resource			21,222			49.4
Process Energy						
Electricity (grid)	159	kwh	1,695	351	kwh	3.95
Electricity (cogeneration)	862	cu ft (2)	887	53.8	cu meters	2.07
Natural gas	3,985	cu ft	4,463	249	cu meters	10.4
LPG	0.034	gal	3.67	0.28	liter	0.0085
Distillate oil	0.18	gal	28.5	1.50	liter	0.066
Residual oil	1.52	gal	261	12.7	liter	0.61
Gasoline	0.11	gal	15.8	0.93	liter	0.037
Diesel	0.0094	gal	1.50	0.079	liter	0.0035
Internal Offgas use (1)						
From Oil	25.8	lb	792	25.8	kg	1.84
From Natural Gas	118	lb	3,608	118	kg	8.40
Recovered Energy	11.9	thousand Btu	11.9	27.6	MJ	0.028
Total Process			11,744			27.3
Transportation Energy						
Combination truck	7.56	ton-miles		24.3	tonne-km	
Diesel	0.079	gal	12.6	0.66	liter	0.029
Rail	6.53	ton-miles		21.0	tonne-km	
Diesel	0.017	gal	2.66	0.14	liter	0.0062
Barge	15.6	ton-miles		50.1	tonne-km	
Diesel	0.013	gal	2.05	0.11	liter	0.0048
Residual oil	0.043	gal	7.35	0.36	liter	0.017
Ocean freighter	315	ton-miles		1,013	tonne-km	
Diesel	0.060	gal	9.50	0.50	liter	0.022
Residual	0.54	gal	92.4	4.49	liter	0.21
Pipeline-natural gas	470	ton-miles		1,512	tonne-km	
Natural gas	324	cu ft	363	20.2	cu meter	0.84
Pipeline-petroleum products	124	ton-miles		398	tonne-km	
Electricity	2.70	kwh	27.6	5.95	kwh	0.064
Total Transportation			517			1.20

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table B-1

DATA FOR THE PRODUCTION
OF HIGH-DENSITY POLYETHYLENE (HDPE) RESIN
(Cradle-to-Resin)
(page 2 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Ammonia	7.5E-04	lb	7.5E-04	kg
Antimony	4.3E-07	lb	4.3E-07	kg
Arsenic	5.4E-08	lb	5.4E-08	kg
Benzene	0.091	lb	0.091	kg
Carbon Dioxide - Fossil	66.2	lb	66.2	kg
Carbon Monoxide	0.25	lb	0.25	kg
Carbon Tetrachloride	2.9E-07	lb	2.9E-07	kg
CFC 13 (Methane, trichlorofluoro-)	4.6E-06	lb	4.6E-06	kg
Chlorine	9.9E-05	lb	9.9E-05	kg
Chromium	1.4E-07	lb	1.4E-07	kg
Ethylbenzene	0.011	lb	0.011	kg
Ethylene Dibromide	9.0E-07	lb	9.0E-07	kg
HCFC-22	9.9E-07	lb	9.9E-07	kg
Hydrogen	0.0039	lb	0.0039	kg
Hydrogen Chloride	9.9E-07	lb	9.9E-07	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.14	lb	0.14	kg
Methane	6.13	lb	6.13	kg
Nickel	1.2E-06	lb	1.2E-06	kg
Nitrogen Oxides	0.12	lb	0.12	kg
Non-Methane Hydrocarbons	0.51	lb	0.51	kg
Other Organics	0.011	lb	0.011	kg
Particulates (PM10)	0.15	lb	0.15	kg
Particulates (PM2.5)	0.017	lb	0.017	kg
Particulates (unspecified)	0.026	lb	0.026	kg
Polyaromatic Hydrocarbons (total)	1.2E-05	lb	1.2E-05	kg
Sulfur Dioxide	1.84	lb	1.84	kg
Sulfur Oxides	0.0041	lb	0.0041	kg
Toluene	0.14	lb	0.14	kg
VOC	0.73	lb	0.73	kg
Xylene	0.082	lb	0.082	kg
Solid Wastes				
Landfilled	32.1	lb	32.1	kg
Burned	3.84	lb	3.84	kg
Waste-to-Energy	0.027	lb	0.027	kg
Waterborne Wastes				
m-Xylene	8.4E-06	lb	8.4E-06	kg
1-Methylfluorene	2.0E-08	lb	2.0E-08	kg
2,4-Dimethylphenol	8.1E-06	lb	8.1E-06	kg
2-Hexanone	1.9E-06	lb	1.9E-06	kg
2-Methylnaphthalene	4.4E-06	lb	4.4E-06	kg
4-Methyl-2-Pentanone	7.4E-07	lb	7.4E-07	kg
Acetone	1.8E-06	lb	1.8E-06	kg
Acid (benzoic)	2.9E-04	lb	2.9E-04	kg
Acid (hexanoic)	6.0E-05	lb	6.0E-05	kg
Alkylated benzenes	5.4E-05	lb	5.4E-05	kg
Alkylated fluorenes	3.1E-06	lb	3.1E-06	kg
Alkylated naphthalenes	8.8E-07	lb	8.8E-07	kg
Alkylated phenanthrenes	3.7E-07	lb	3.7E-07	kg
Aluminum	0.027	lb	0.027	kg
Ammonia	0.0062	lb	0.0062	kg
Antimony	1.7E-05	lb	1.7E-05	kg
Arsenic	5.4E-05	lb	5.4E-05	kg
Barium	0.36	lb	0.36	kg
Benzene	3.1E-04	lb	3.1E-04	kg
Beryllium	3.4E-06	lb	3.4E-06	kg
BOD	0.042	lb	0.042	kg
Boron	9.0E-04	lb	9.0E-04	kg
Bromide	0.035	lb	0.035	kg
Cadmium	8.4E-06	lb	8.4E-06	kg
Calcium	0.58	lb	0.58	kg
Chlorides	7.25	lb	7.25	kg

Table B-1

DATA FOR THE PRODUCTION
OF HIGH-DENSITY POLYETHYLENE (HDPE) RESIN
(Cradle-to-Resin)
(page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Chromium (unspecified)	7.2E-04	lb	7.2E-04	kg
Cobalt	6.4E-06	lb	6.4E-06	kg
COD	0.11	lb	0.11	kg
Copper	7.7E-05	lb	7.7E-05	kg
Cyanide	1.3E-08	lb	1.3E-08	kg
Dibenzofuran	3.3E-08	lb	3.3E-08	kg
Dibenzothiophene	2.7E-08	lb	2.7E-08	kg
Dissolved Solids	7.31	lb	7.31	kg
Ethylbenzene	2.7E-05	lb	2.7E-05	kg
Fluorene	1.5E-06	lb	1.5E-06	kg
Furans	1.0E-06	lb	1.0E-06	kg
Hydrocarbons	0.0010	lb	0.0010	kg
Iron	0.049	lb	0.049	kg
Lead	1.4E-04	lb	1.4E-04	kg
Lead 210	3.0E-14	lb	3.0E-14	kg
Lithium	0.14	lb	0.14	kg
Magnesium	0.12	lb	0.12	kg
Manganese	1.7E-04	lb	1.7E-04	kg
Mercury	3.0E-07	lb	3.0E-07	kg
Methyl Chloride	7.1E-09	lb	7.1E-09	kg
Methyl Ethyl Ketone	1.4E-08	lb	1.4E-08	kg
Molybdenum	6.6E-06	lb	6.6E-06	kg
Naphthalene	5.2E-06	lb	5.2E-06	kg
n-Decane	8.4E-06	lb	8.4E-06	kg
n-Docosane	1.9E-07	lb	1.9E-07	kg
n-Dodecane	1.6E-05	lb	1.6E-05	kg
n-Eicosane	4.3E-06	lb	4.3E-06	kg
n-Hexacosane	1.2E-07	lb	1.2E-07	kg
n-Hexadecane	1.7E-05	lb	1.7E-05	kg
Nickel	6.6E-05	lb	6.6E-05	kg
n-Octadecane	4.3E-06	lb	4.3E-06	kg
p -Xylene	3.1E-06	lb	3.1E-06	kg
o -Xylene	3.1E-06	lb	3.1E-06	kg
o-Cresol	8.3E-06	lb	8.3E-06	kg
Oil	0.012	lb	0.012	kg
p-Cresol	8.9E-06	lb	8.9E-06	kg
p-Cymene	1.8E-08	lb	1.8E-08	kg
Pentamethylbenzene	1.3E-08	lb	1.3E-08	kg
Phenanthrene	2.3E-07	lb	2.3E-07	kg
Phenol/ Phenolic Compounds	0.0011	lb	0.0011	kg
Phosphorus	1.0E-04	lb	1.0E-04	kg
Process solvents	1.0E-04	lb	1.0E-04	kg
Tetradecane	6.8E-06	lb	6.8E-06	kg
Radium 226	1.0E-11	lb	1.0E-11	kg
Radium 228	5.3E-14	lb	5.3E-14	kg
Selenium	3.5E-06	lb	3.5E-06	kg
Silver	3.5E-04	lb	3.5E-04	kg
Sodium	1.66	lb	1.66	kg
Strontium	0.016	lb	0.016	kg
Styrene	9.9E-07	lb	9.9E-07	kg
Sulfates	0.012	lb	0.012	kg
Sulfides	3.9E-05	lb	3.9E-05	kg
Sulfur	7.2E-04	lb	7.2E-04	kg
Surfactants	1.4E-04	lb	1.4E-04	kg
Suspended Solids	2.97	lb	2.97	kg
Thallium	3.5E-06	lb	3.5E-06	kg
Tin	6.6E-05	lb	6.6E-05	kg
Titanium	2.5E-04	lb	2.5E-04	kg
TOC	0.0010	lb	0.0010	kg
Toluene	3.8E-04	lb	3.8E-04	kg
Total biphenyls	3.5E-06	lb	3.5E-06	kg
Total dibenzothiophenes	1.1E-08	lb	1.1E-08	kg
Vanadium	1.9E-05	lb	1.9E-05	kg
Xylene, unspecified	1.3E-04	lb	1.3E-04	kg
Yttrium	1.9E-06	lb	1.9E-06	kg
Zinc	6.8E-04	lb	6.8E-04	kg

References: Tables B-2 through B-7

Source: Franklin Associates, A Division of ERG models

Crude Oil Production

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

There are two primary sources of waste from crude oil production. The first source is the "oil field brine," or water that is extracted with the oil. The brine goes through a separator at or near the well head in order to remove the oil from the water. These separators are very efficient and leave minimal oil in the water.

According to the American Petroleum Institute, 17.9 billion barrels of brine water were produced from crude oil production in 1995 (Reference B-2). This equates to a ratio of 5.4 barrels of water per barrel of oil. The majority of this brine is produced by onshore oil production facilities. Only a small percentage of onshore brine is discharged to surface water. The majority is injected into wells specifically designed for production-related waters (Reference B-3). The remaining brine is produced from offshore oil production facilities, and most of this is released to the ocean (Reference B-46). Therefore, all waterborne wastes from crude oil production are attributable to the water released from offshore production (Reference B-4). Because crude oil is frequently produced along with natural gas, a portion of the data is allocated to natural gas production (Reference B-2).

Evolving technologies are reducing the amount of brine that is extracted during oil recovery and minimizing the environmental impact of discharged brine. For example, downhole separation is a technology that separates brine from oil before bringing it to the surface; the brine is injected into subsurface injection zones. The freeze-thaw evaporation (FTE) process is another technology that reduces the discharge of brine water by using a freeze crystallization process in the winter and a natural evaporation process in the summer to extract fresh water from brine water; the fresh water can be used for horticulture or agriculture applications (Reference B-5).

There are also waterborne emissions associated with drilling wastes. Suspensions of solids, chemicals, and other materials in a base of water, oil, or synthetic-based material are referred to as drilling fluids or drilling muds. These are formulated to lubricate and cool the drill bit, carry drill cuttings from the hole to the surface, and maintain downhole hydrostatic pressure. (Reference B-44). The volume of drilling waste is small in comparison to oil field brine (Reference B-2). Less than 1% of drilling fluids from onshore production are discharged to water, while about 90% of offshore drilling fluids are discharged (References B-45, B-46). Toxic metal pollutants are released due to the use of barite, which is employed to control the density of drilling fluids. (Reference B-44).

The primary source of atmospheric process emissions from oil extraction operations is gas produced from oil wells. The majority of this gas is recovered for sale, but some is released to the atmosphere. Atmospheric emissions from crude oil production are primarily hydrocarbons, attributed to the natural gas produced from combination wells and relate to line or transmission losses and unflared venting. Carbon dioxide is also released, primarily from storage tank venting. The amount of methane released from crude oil production was calculated from EPA's Inventory of U.S. Greenhouse Gas Emissions and Sinks, which has data specific to oil field emissions (Reference B-6).

The requirements for transporting crude oil from the production field to the Gulf Coast of the United States (where most petroleum refining in the United States occurs) were calculated from foreign and domestic supply data, port-to-port distance data, and domestic petroleum movement data (References B-7 and B-8). Based on 2001 foreign and domestic supply data, 62 percent of the United States crude oil supply is from foreign sources, 6 percent is from Alaska, and the remaining 32 percent is from the lower 48 states. These percentages were used to apportion transportation requirements among different transportation modes. With the exception of Canada, which transports crude oil to the United States by pipeline, foreign suppliers transport crude oil to the United States by ocean tanker. (In 2001, Saudi Arabia, Mexico, Canada, Venezuela, and Nigeria were the top five foreign suppliers of crude oil to the United States.) The transportation of crude oil from Alaska to the lower 48 states is also accomplished by ocean tanker. Domestic transportation of crude oil is accomplished by pipeline and barge.

Table B-2 shows the energy requirements and emissions for the extraction of crude oil.

Distillation, Desalting, and Hydrotreating

Gasoline and diesel are the primary outputs from refineries; however, other major products include kerosene, aviation fuel, residual oil, lubricating oil, and feedstocks for the petrochemical industry. Data specific to the production of each type of refinery product are not available. Such data would be difficult to characterize because there are many types of conversion processes in oil refineries that are altered depending on market demand, quality of crude input, and other variables. Thus, the following discussion is applicable to all refinery products.

A petroleum refinery processes crude oil into thousands of products using physical and/or chemical processing technology. A petroleum refinery receives crude oil, which is comprised of mixtures of many hydrocarbon compounds and uses distillation processes to separate pure product streams. Because the crude oil is contaminated (to varying degrees) with compounds of sulfur, nitrogen, oxygen, and metals, cleaning operations are common in all refineries. Also, the natural hydrocarbon components that comprise crude oil are often chemically changed to yield products for which there is higher demand. These processes, such as polymerization, alkylation, reforming, and visbreaking, are used to convert light or heavy crude oil fractions into intermediate weight products, which are more easily handled and used as fuels and/or feedstocks (Reference B-18).

Table B-2

DATA FOR THE EXTRACTION OF CRUDE OIL
(page 1 of 2)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Petroleum	1,035	lb	18,770	1,035	kg	43.7
Total Resource			18,770			43.7
Process Energy						
Electricity (grid)	17.7	kwh	188	39.0	kwh	0.44
Natural gas	525	cu ft	588	32.8	cu meters	1.37
Distillate oil	0.15	gal	24.6	1.29	liter	0.057
Residual oil	0.10	gal	16.4	0.80	liter	0.038
Gasoline	0.082	gal	11.7	0.68	liter	0.027
Total Process			829			1.93
Transportation Energy						
Barge	0.37	ton-miles		1.21	tonne-km	
Diesel	3.0E-04	gal	0.048	0.0025	liter	1.1E-04
Residual oil	0.0010	gal	0.17	0.0083	liter	4.0E-04
Ocean freighter	1,472	ton-miles		4,738	tonne-km	
Diesel	0.28	gal	44.4	2.33	liter	0.10
Residual	2.52	gal	432	21.0	liter	1.00
Pipeline-petroleum products	196	ton-miles		631	tonne-km	
Electricity	4.27	kwh	43.8	9.42	kwh	0.10
Total Transportation			520			1.21
Environmental Emissions						
Atmospheric Emissions						
Methane	5.27	lb		5.27	kg	
Carbon Dioxide	1.11	lb		1.11	kg	
Solid Wastes						
Landfilled	26.1	lb		26.1	kg	
Waterborne Wastes						
2-Hexanone	1.4E-06	lb		1.4E-06	kg	
4-Methyl-2-Pentanone	1.9E-07	lb		1.9E-07	kg	
Acetone	4.6E-07	lb		4.6E-07	kg	
Aluminum	0.021	lb		0.021	kg	
Ammonia	0.0028	lb		0.0028	kg	
Antimony	1.3E-05	lb		1.3E-05	kg	
Arsenic, ion	4.6E-05	lb		4.6E-05	kg	
Barium	0.28	lb		0.28	kg	
Benzene	2.6E-04	lb		2.6E-04	kg	
Benzene, 1-methyl-4-(1-methylethyl)-	4.6E-09	lb		4.6E-09	kg	
Benzene, ethyl-	1.4E-05	lb		1.4E-05	kg	
Benzene, pentamethyl-	3.4E-09	lb		3.4E-09	kg	
Benzenes, alkylated, unspecified	4.3E-05	lb		4.3E-05	kg	
Benzoic acid	2.2E-04	lb		2.2E-04	kg	
Beryllium	2.9E-06	lb		2.9E-06	kg	
Biphenyl, total	2.8E-06	lb		2.8E-06	kg	
BOD5, Biological Oxygen Demand	0.025	lb		0.025	kg	
Boron	6.9E-04	lb		6.9E-04	kg	
Bromide	0.031	lb		0.031	kg	
Cadmium, ion	7.1E-06	lb		7.1E-06	kg	
Calcium, ion	0.50	lb		0.50	kg	
Chloride	6.07	lb		6.07	kg	
Chromium	5.6E-04	lb		5.6E-04	kg	
Cobalt	4.9E-06	lb		4.9E-06	kg	
COD, Chemical Oxygen Demand	0.042	lb		0.042	kg	
Copper, ion	6.2E-05	lb		6.2E-05	kg	
Cyanide	3.3E-09	lb		3.3E-09	kg	
Decane	6.4E-06	lb		6.4E-06	kg	

Table B-2

DATA FOR THE EXTRACTION OF CRUDE OIL

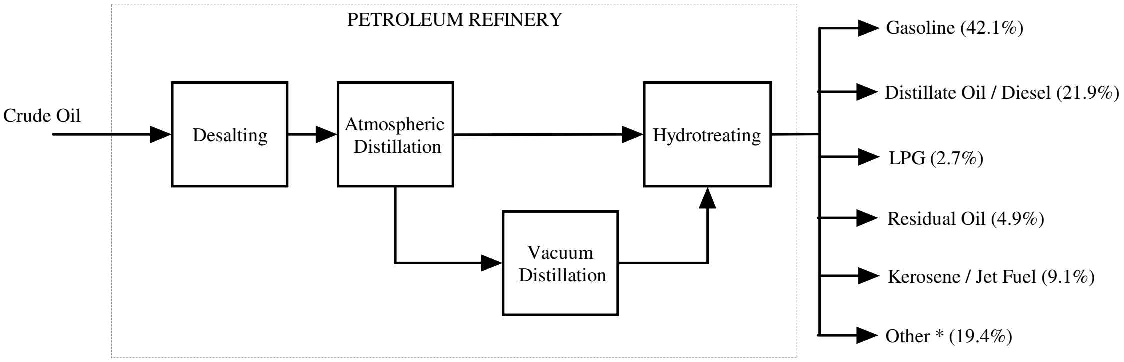
(page 2 of 2)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Dibenzofuran	8.7E-09	lb	8.7E-09	kg
Dibenzothiophene	7.0E-09	lb	7.0E-09	kg
Dibenzothiophene, total	8.6E-09	lb	8.6E-09	kg
Dissolved solids	6.47	lb	6.47	kg
Docosane	4.9E-08	lb	4.9E-08	kg
Dodecane	1.2E-05	lb	1.2E-05	kg
Eicosane	3.3E-06	lb	3.3E-06	kg
Florene, 1-methyl-	5.2E-09	lb	5.2E-09	kg
Florenes, alkylated, unspecified	2.5E-06	lb	2.5E-06	kg
Fluorine	1.2E-06	lb	1.2E-06	kg
Hexadecane	1.3E-05	lb	1.3E-05	kg
Hexanoic acid	4.7E-05	lb	4.7E-05	kg
Iron	0.039	lb	0.039	kg
Lead	1.2E-04	lb	1.2E-04	kg
Lead-210/kg	2.3E-14	lb	2.3E-14	kg
Lithium, ion	1.6E-04	lb	1.6E-04	kg
Magnesium	0.10	lb	0.10	kg
Manganese	1.5E-04	lb	1.5E-04	kg
Methane, monochloro-, R-40	1.8E-09	lb	1.8E-09	kg
Methyl ethyl ketone	3.7E-09	lb	3.7E-09	kg
Molybdenum	5.1E-06	lb	5.1E-06	kg
m-Xylene	6.3E-06	lb	6.3E-06	kg
Naphthalene	4.0E-06	lb	4.0E-06	kg
Naphthalenes, alkylated, unspecified	7.0E-07	lb	7.0E-07	kg
Napthalene, 2-methyl-	3.3E-06	lb	3.3E-06	kg
n-Hexacosane	3.0E-08	lb	3.0E-08	kg
Nickel	5.4E-05	lb	5.4E-05	kg
o-Cresol	6.4E-06	lb	6.4E-06	kg
Oils, unspecified	0.0043	lb	0.0043	kg
o-xylene	2.3E-06	lb	2.3E-06	kg
p-Cresol	6.9E-06	lb	6.9E-06	kg
Phenanthrene	1.8E-07	lb	1.8E-07	kg
Phenanthrenes, alkylated, unspecified	2.9E-07	lb	2.9E-07	kg
Phenol	7.2E-05	lb	7.2E-05	kg
Phenol, 2,4-dimethyl-	6.2E-06	lb	6.2E-06	kg
p-xylene	2.3E-06	lb	2.3E-06	kg
Radium-226/kg	8.0E-12	lb	8.0E-12	kg
Radium-228/kg	4.1E-14	lb	4.1E-14	kg
Selenium	2.5E-06	lb	2.5E-06	kg
Silver	3.1E-04	lb	3.1E-04	kg
Sodium, ion	1.48	lb	1.48	kg
Strontium	0.012	lb	0.012	kg
Sulfate	0.011	lb	0.011	kg
Sulfur	5.3E-04	lb	5.3E-04	kg
Surfactants	1.2E-04	lb	1.2E-04	kg
Suspended solids, unspecified	2.32	lb	2.32	kg
Tetradecane	5.1E-06	lb	5.1E-06	kg
Thallium	2.8E-06	lb	2.8E-06	kg
Tin	5.2E-05	lb	5.2E-05	kg
Titanium, ion	2.0E-04	lb	2.0E-04	kg
Toluene	2.4E-04	lb	2.4E-04	kg
Vanadium	5.7E-06	lb	5.7E-06	kg
Xylene	1.2E-04	lb	1.2E-04	kg
Yttrium	1.5E-06	lb	1.5E-06	kg
Zinc	4.8E-04	lb	4.8E-04	kg

References: B-2, B-6, B-8 through B-17, and B-44 through B-47.

Source: Franklin Associates, A Division of ERG

This module includes data for desalting, atmospheric distillation, vacuum distillation, and hydrotreating. These are the most energy-intensive processes of a petroleum refinery, representing over 95 percent of the total energy requirements of U.S. petroleum refineries (Reference B-19). Data for cracking, reforming, and supporting processes are not available and are not included in this module. The following figure is a simplified flow diagram of the material flows and processes included in this module.



Simplified flow diagram for petroleum refinery operations for the production of fuels.
All arrows represent material flows. The percentages of refinery products represent percent by mass of total refinery output.
* "Other" category includes still gas, petroleum coke, asphalt, and petrochemical feedstocks .

Air pollution is caused by various petroleum refining processes, including vacuum distillation, catalytic cracking, thermal cracking processes, and sulfur recovery. Fugitive emissions also contribute significantly to air emissions. Fugitive emissions include leaks from valves, seals, flanges, and drains, as well as leaks escaping from storage tanks or during transfer operations. The wastewater treatment plant for a refinery is also a source of fugitive emissions (Reference B-20). Emissions of atmospheric and waterborne emissions for petroleum refineries were derived from U.S. EPA and Department of Energy publications (References B-47, B-51, B-52, B-53, B-54).

This module expresses data on the basis 1,000 pounds of general refinery product as well as data allocated to specific refinery products. The data are allocated to specific refinery products based on the percent by mass of each product in the refinery output. The mass allocation method assigns energy requirements and environmental emissions equally to all refinery products -- equal masses of different refinery products are assigned equal energy and emissions.

Mass allocation is not the only method that can be used for assigning energy and emissions to refinery products. Heat of combustion and economic value are two additional methods for co-product allocation. Using heat of combustion of refinery products yields allocation factors similar to those derived by mass allocation, demonstrating the correlation between mass and heat of combustion. Economic allocation is complicated because market values fluctuate with supply and demand, and market data are not available for refinery products such as asphalt. This module does not apply the heat of combustion or economic allocation methods because they have no apparent advantage over mass allocation.

Co-product function expansion is yet another method for allocating environmental burdens among refinery products. Co-product function expansion is more complex than mass, heat of combustion, or economic allocation; it evaluates downstream processes and product substitutes in order to determine the percentage of total energy and emissions to assign to each refinery product. This module does not use the co-product function expansion method because it is outside the scope of this project.

There are advantages and disadvantages for each type of allocation method. Until detailed data are available for the material flows and individual processes within a refinery, life cycle practitioners will have to resort to allocation methods such as those discussed above.

The energy requirements and emissions for the refining of petroleum are found in Table B-3.

Natural Gas Production

Natural gas is a widely used energy resource, since it is a relatively clean, efficient, and versatile fuel. The major component of natural gas is methane (CH_4). Other components of natural gas include ethane, propane, butane, and other heavier hydrocarbons, as well as water vapor, carbon dioxide, nitrogen, and hydrogen sulfides.

Natural gas is extracted from deep underground wells and is frequently co-produced with crude oil. Because of its gaseous nature, natural gas flows quite freely from wells which produce primarily natural gas, but some energy is required to pump natural gas and crude oil mixtures to the surface. An estimated 80 percent of natural gas is extracted onshore and 20 percent is extracted offshore (Reference B-12).

Atmospheric emissions from natural gas production result primarily from unflared venting. Methane and non-combustion carbon dioxide emissions from natural gas extraction are generally process related, with the largest source of these emissions from normal operations, system upsets, and routine maintenance. Waterborne wastes result from brines that occur when natural gas is produced in combination with oil. In cases where data represent both crude oil and natural gas extraction, the data module allocates environmental emissions based on the percent weight of natural gas produced. The data module also apportions environmental emissions according to the percent share of onshore and offshore extraction.

Energy data for natural gas production were calculated from fuel consumption data for the crude oil and natural gas extraction industry (Reference B-21). The energy and emissions data for the production of natural gas is displayed in Table B-4.

Table B-3

DATA FOR THE REFINING OF PETROLEUM PRODUCTS

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Crude Oil	1,018	lb		1,018	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	64.9	kwh	691	143	kwh	1.61
Natural gas	178	cu ft	199	11.1	cu meters	0.46
LPG	0.14	gal	14.9	1.15	liter	0.035
Residual oil	3.26	gal	560	27.2	liter	1.30
Total Process			1,465			3.41
Transportation Energy						
Combination truck	13.6	ton-miles		43.9	tonne-km	
Diesel	0.14	gal	22.8	1.20	liter	0.053
Rail	8.70	ton-miles		28.0	tonne-km	
Diesel	0.022	gal	3.43	0.18	liter	0.0080
Barge	73.7	ton-miles		237	tonne-km	
Diesel	0.059	gal	9.37	0.49	liter	0.022
Residual oil	0.20	gal	33.7	1.64	liter	0.078
Pipeline-petroleum products	107	ton-miles		345	tonne-km	
Electricity	2.34	kwh	23.9	5.15	kwh	0.056
Total Transportation			93.1			0.22
Environmental Emissions						
Atmospheric Emissions						
Ammonia	0.0036	lb		0.0036	kg	
Antimony	2.0E-06	lb		2.0E-06	kg	
Arsenic	2.6E-07	lb		2.6E-07	kg	
Benzene	0.0011	lb		0.0011	kg	
Carbon dioxide, fossil	0.25	lb		0.25	kg	
Carbon monoxide	0.42	lb		0.42	kg	
Chromium	6.8E-07	lb		6.8E-07	kg	
Ethylene dibromide	4.3E-06	lb		4.3E-06	kg	
Methane, chlorotrifluoro-, CFC-13	2.2E-05	lb		2.2E-05	kg	
Methane, fossil	0.037	lb		0.037	kg	
Methane, tetrachloro-, CFC-10	1.4E-06	lb		1.4E-06	kg	
Nickel	5.8E-06	lb		5.8E-06	kg	
Nitrogen oxides	0.42	lb		0.42	kg	
NMVOC, non-methane volatile organic compounds, unspecified origin	0.68	lb		0.68	kg	
Particulates, < 10 um	0.031	lb		0.031	kg	
Particulates, < 2.5 um	0.023	lb		0.023	kg	
Polycyclic organic matter, unspecified	5.6E-05	lb		5.6E-05	kg	
SO2	0.25	lb		0.25	kg	
Solid Wastes						
Landfilled	5.60	lb		5.60	kg	
Waterborne Emissions						
Ammonia	0.015	lb		0.015	kg	
BOD5, Biological Oxygen Demand	0.034	lb		0.034	kg	
Chromium	3.0E-06	lb		3.0E-06	kg	
COD, Chemical Oxygen Demand	0.23	lb		0.23	kg	
Lead	9.8E-07	lb		9.8E-07	kg	
Mercury	6.0E-08	lb		6.0E-08	kg	
Oils, unspecified	0.011	lb		0.011	kg	
Phenol	2.3E-04	lb		2.3E-04	kg	
Selenium	1.6E-06	lb		1.6E-06	kg	
Sulfide	1.9E-04	lb		1.9E-04	kg	
Suspended solids, unspecified	0.028	lb		0.028	kg	
Vanadium	5.4E-05	lb		5.4E-05	kg	

References: B-6, B-16, B-17, and B-22 through B-26

Source: Franklin Associates, A Division of ERG

Table B-4

DATA FOR THE EXTRACTION OF NATURAL GAS
(page 1 of 2)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas	1,038	lb	21,416	1,038	kg	49.8
Total Resource			21,416			49.8
Process Energy						
Electricity (grid)	17.7	kwh	188	39.0	kwh	0.44
Natural gas	525	cu ft	588	32.8	cu meters	1.37
Distillate oil	0.15	gal	24.6	1.29	liter	0.057
Residual oil	0.10	gal	16.4	0.8	liter	0.038
Gasoline	0.082	gal	11.7	0.68	liter	0.027
Total Process			829			1.93
Environmental Emissions						
Atmospheric Emissions						
Methane	3.40	lb		3.40	kg	
Carbon dioxide (fossil)	17.0	lb		17.0	kg	
Solid Wastes						
Landfilled	26.1	lb		26.1	kg	
Waterborne Wastes						
2-Hexanone	1.7E-06	lb		1.7E-06	kg	
4-Methyl-2-Pentanone	7.4E-07	lb		7.4E-07	kg	
Acetone	1.8E-06	lb		1.8E-06	kg	
Aluminum	0.023	lb		0.023	kg	
Ammonia	0.0025	lb		0.0025	kg	
Antimony	1.4E-05	lb		1.4E-05	kg	
Arsenic, ion	4.7E-05	lb		4.7E-05	kg	
Barium	0.31	lb		0.31	kg	
Benzene	2.6E-04	lb		2.6E-04	kg	
Benzene, 1-methyl-4-(1-methylethyl)-	1.8E-08	lb		1.8E-08	kg	
Benzene, ethyl-	1.5E-05	lb		1.5E-05	kg	
Benzene, pentamethyl-	1.3E-08	lb		1.3E-08	kg	
Benzenes, alkylated, unspecified	4.7E-05	lb		4.7E-05	kg	
Benzoic acid	2.6E-04	lb		2.6E-04	kg	
Beryllium	3.0E-06	lb		3.0E-06	kg	
Biphenyl	3.1E-06	lb		3.1E-06	kg	
BOD5, Biological Oxygen Demand	0.024	lb		0.024	kg	
Boron	8.0E-04	lb		8.0E-04	kg	
Bromide	0.030	lb		0.030	kg	
Cadmium, ion	7.3E-06	lb		7.3E-06	kg	
Calcium, ion	0.50	lb		0.50	kg	
Chloride	6.30	lb		6.30	kg	
Chromium	6.2E-04	lb		6.2E-04	kg	
Cobalt	5.6E-06	lb		5.6E-06	kg	
COD, Chemical Oxygen Demand	0.040	lb		0.040	kg	
Copper, ion	6.7E-05	lb		6.7E-05	kg	
Cyanide	1.3E-08	lb		1.3E-08	kg	
Decane	7.4E-06	lb		7.4E-06	kg	
Dibenzofuran	3.3E-08	lb		3.3E-08	kg	
Dibenzothiophene	2.7E-08	lb		2.7E-08	kg	
Dibenzothiophene, total	9.4E-09	lb		9.4E-09	kg	
Dissolved solids	6.23	lb		6.23	kg	
Docosane	1.9E-07	lb		1.9E-07	kg	
Dodecane	1.4E-05	lb		1.4E-05	kg	

Table B-4

DATA FOR THE EXTRACTION OF NATURAL GAS
(page 2 of 2)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Eicosane	3.9E-06	lb	3.9E-06	kg
Florene, 1-methyl-	2.0E-08	lb	2.0E-08	kg
Florenes, alkylated, unspecified	2.7E-06	lb	2.7E-06	kg
Fluorine	1.3E-06	lb	1.3E-06	kg
Hexadecane	1.5E-05	lb	1.5E-05	kg
Hexanoic acid	5.3E-05	lb	5.3E-05	kg
Iron	0.043	lb	0.043	kg
Lead	1.3E-04	lb	1.3E-04	kg
Lead-210/kg	2.6E-14	lb	2.6E-14	kg
Lithium, ion	0.15	lb	0.15	kg
Magnesium	0.10	lb	0.10	kg
Manganese	1.4E-04	lb	1.4E-04	kg
Methane, monochloro-, R-40	7.1E-09	lb	7.1E-09	kg
Methyl ethyl ketone	1.4E-08	lb	1.4E-08	kg
Molybdenum	5.8E-06	lb	5.8E-06	kg
m-Xylene	7.5E-06	lb	7.5E-06	kg
Naphthalene	4.6E-06	lb	4.6E-06	kg
Naphthalenes, alkylated, unspecified	7.7E-07	lb	7.7E-07	kg
Napthalene, 2-methyl-	3.9E-06	lb	3.9E-06	kg
n-Hexacosane	1.2E-07	lb	1.2E-07	kg
Nickel	5.8E-05	lb	5.8E-05	kg
o-Cresol	7.3E-06	lb	7.3E-06	kg
Oils, unspecified	0.0045	lb	0.0045	kg
o-xylene	2.8E-06	lb	2.8E-06	kg
p-Cresol	7.9E-06	lb	7.9E-06	kg
Phenanthrene	2.0E-07	lb	2.0E-07	kg
Phenanthrenes, alkylated, unspecified	3.2E-07	lb	3.2E-07	kg
Phenols, unspecified	7.4E-05	lb	7.4E-05	kg
Phenol, 2,4-dimethyl-	7.1E-06	lb	7.1E-06	kg
p-xylene	2.8E-06	lb	2.8E-06	kg
Radium-226/kg	9.2E-12	lb	9.2E-12	kg
Radium-228/kg	4.7E-14	lb	4.7E-14	kg
Selenium	2.8E-06	lb	2.8E-06	kg
Silver	3.0E-04	lb	3.0E-04	kg
Sodium, ion	1.43	lb	1.43	kg
Strontium	0.014	lb	0.014	kg
Sulfate	0.010	lb	0.010	kg
Sulfur	6.5E-04	lb	6.5E-04	kg
Surfactants, unspecified	1.2E-04	lb	1.2E-04	kg
Suspended solids, unspecified	2.56	lb	2.56	kg
Tetradecane	6.0E-06	lb	6.0E-06	kg
Thallium	3.1E-06	lb	3.1E-06	kg
Tin	5.8E-05	lb	5.8E-05	kg
Titanium, ion	2.2E-04	lb	2.2E-04	kg
Toluene	2.4E-04	lb	2.4E-04	kg
Vanadium	6.8E-06	lb	6.8E-06	kg
Xylene	1.1E-04	lb	1.1E-04	kg
Yttrium	1.7E-06	lb	1.7E-06	kg
Zinc	5.3E-04	lb	5.3E-04	kg

References: B-2, B-6, B-8 through B-17, and B-44 through B-47

Source: Franklin Associates, A Division of ERG

Natural Gas Processing

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

Atmospheric emissions result from acid gas removal processes and flaring of hydrogen sulfide (H2S), the regeneration of glycol solutions, and fugitive emissions of methane. Methane and carbon dioxide emissions from natural gas processing were calculated based on emissions reported in the U.S. Greenhouse Gas Inventory . For natural gas that is sweetened, the majority of the H_2S removed is used for production of sulfur (Reference B-48). Sulfur dioxide emissions were calculated for flaring of H_2S that is not used for recovered sulfur production (Reference B-49). . Glycol solutions are used to dehydrate natural gas, and the regeneration of these solutions result in the release of BTEX (benzene, toluene, ethylbenzene, and xylene) as well as a variety of less toxic organics (Reference B-28, B-50). Negligible particulate emissions are produced from natural gas plants, and the relatively low processing temperatures (<1,200 degrees Fahrenheit) prevent the formation of nitrogen oxides (NOx).

Natural gas is transported primarily by pipeline, but a small percentage is compressed and transported by insulated railcars and tankers (References B-30 and B-31). Transportation data were calculated from the net annual quantities of natural gas imported and exported by each state (Reference B-32).

Energy data for natural gas processing were calculated from fuel consumption data for the natural gas liquids extraction industry (Reference B-9). Table B-5 shows the energy and emissions data for processing natural gas. Sulfur was given no coproduct allocation in this process. The amount of H_2S in the sour natural gas varies widely depending on where it is extracted.

Olefins Production (Ethylene)

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

Typical production of ethylene, propylene, and other coproducts begins when hydrocarbons and steam are fed to the cracking furnace. After being heated to temperatures around 1,000° Celsius, the cracked products are quenched in heat exchangers which produce high pressure steam. Fuel oil is separated from the main gas stream in a multi-stage centrifugal compressor. The main gas stream then undergoes hydrogen sulfide removal and drying. The final step involves fractional distillation of the various reaction products.

Table B-5

**DATA FOR THE PROCESSING OF
NATURAL GAS**

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Natural gas	1,005	lb		1,005	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	9.67	kwh	103	21.3	kwh	0.24
Natural gas	554	cu ft	620	34.6	cu meters	1.44
Distillate oil	0.0060	gal	0.96	0.050	liter	0.0022
Residual oil	0.0059	gal	1.02	0.050	liter	0.0024
Gasoline	0.0057	gal	0.81	0.048	liter	0.0019
Total Process			726			1.69
Transportation Energy						
Combination truck	5.00	ton-miles		16.1	tonne-km	
Diesel	0.052	gal	8.33	0.44	liter	0.019
Rail	5.00	ton-miles		16.1	tonne-km	
Diesel	0.012	gal	1.97	0.10	liter	0.0046
Pipeline-natural gas	500	ton-miles		1,608	tonne-km	
Natural gas	345	cu ft	386	21.5	cu meter	0.90
Total Transportation			397			0.92
Environmental Emissions						
Atmospheric Emissions						
BTEX	0.34	lb		0.34	kg	
Benzene	0.096	lb		0.096	kg	
Toluene	0.15	lb		0.15	kg	
Ethylbenzene	0.012	lb		0.012	kg	
Xylene	0.087	lb		0.087	kg	
Methane	1.88	lb		1.88	kg	
SO2	1.90	lb		1.90	kg	
VOC	0.77	lb		0.77	kg	
Carbon Dioxide	53.0	lb		53.0	kg	

References: B-9 through B-12, B-17, B-26 through B-31, and B-33.

Source: Franklin Associates, A Division of ERG

Within the hydrocracker, an offgas is produced from the raw materials entering. A portion of this offgas is used within the hydrocracker to produce steam, while the remaining portion is exported from the hydrocracker as a coproduct, as discussed below. The offgas used within the hydrocracker is shown in Table B-6 as “Internal offgas use.” This offgas is shown as a weight of natural gas and petroleum input to produce the energy, as well as the energy amount produced from those weights.

Data was collected from individual plants, and a mass allocation was used to provide an output of 1,000 pounds/kilograms of olefin product. Then a weighted average using ethylene production amounts for each plant was applied to the individual olefins plant production data collected from three leading producers (8 thermal cracking units) in North America. Transportation amounts for ethylene were calculated using a weighted average of data collected from the polyethylene producers. Numerous coproduct streams are produced during this process. Fuel gas and off-gas were two of the coproducts produced that were exported to another process for fuel use. When these fuel coproducts are exported from the hydrocracker, they carry with them the allocated share of the inputs and outputs for their production. The ratio of the mass of the exported fuel over the total mass output was removed from the total inputs and outputs of the hydrocracker, and the remaining inputs and outputs are allocated over the material hydrocracker products (Equation 1).

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

where
IO = Input/Output Matrix to produce all products/coproducts
M_{EO} = Mass of Exported Offgas
M_{Total} = Mass of all Products and Coproducts (including fuels)

No energy credit is applied for the exported fuels, since both the inputs and outputs for the exported fuels have been removed from the data set. Table B-6 shows the averaged energy and emissions data for the production of ethylene.

As of 2003, there were 16 olefin producers and at least 29 olefin plants in the U.S. (Reference B-42). While data was collected from a relatively small sample of plants, the olefins producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American olefins production. All data collected were individually reviewed by the data providers.

To assess the quality of the data collected for olefins, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for olefins include direct measurements, information provided by purchasing and utility records, and estimates. The standard production technology for olefins is the steam cracking of hydrocarbons (including natural gas liquids and petroleum liquids). The data in this module represent steam cracking of natural gas and petroleum. All data submitted for olefins represent the year 2003 and U.S. and Canada production.

Table B-6

DATA FOR THE PRODUCTION OF ETHYLENE

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs (1)							
Refined Petroleum Products	186	lb			186	kg	
Processed Natural Gas	830	lb			830	kg	
Water Consumption	195	gal			1,627	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	35.7	kwh		380	78.8	kwh	0.88
Electricity (cogeneration)	202	cu ft	(3)	227	12.6	cu meters	0.53
Natural Gas	2,272	cu ft		2,545	142	cu meters	5.92
Gasoline	0.011	gal		1.56	0.091	liter	0.0036
Diesel	0.0095	gal		1.51	0.079	liter	0.0035
Internal Offgas use (2)							
From Oil	26.1	lb		800	26.1	kg	1.86
From Natural Gas	119	lb		3,645	119	kg	8.49
Recovered Energy	12.4	thousand Btu		12.4	29	MJ	0.029
Total Process				7,587			17.7
Transportation Energy							
Ethylene Products							
Pipeline-Petroleum Products	60.0	ton-miles			193	tonne-km	
Electricity	1.31	kwh		13.4	2.88	kwh	0.031
Environmental Emissions							
Atmospheric Emissions - Process							
Carbon Monoxide	0.0010	lb	(4)		0.0010	kg	
Chlorine	1.0E-04	lb	(4)		1.0E-04	kg	
HCFC-022	1.0E-06	lb	(4)		1.0E-06	kg	
Hydrogen Chloride	1.0E-06	lb	(4)		1.0E-06	kg	
Hydrogen	0.0040	lb			0.0040	kg	
Hydrocarbons (NM)	0.091	lb			0.091	kg	
Methane	0.0010	lb	(4)		0.0010	kg	
Other Organics	0.0010	lb	(4)		0.0010	kg	
Particulates (unspecified)	0.0084	lb			0.0084	kg	
Particulates (PM10)	0.10	lb	(4)		0.10	kg	
Sulfur Oxides	0.0041	lb			0.0041	kg	
VOC	0.010	lb	(4)		0.010	kg	
Atmospheric Emissions - Fuel-Related (5)							
Carbon Dioxide (fossil)	648	lb			648	kg	
Carbon Monoxide	0.39	lb			0.39	kg	
Nitrogen Oxides	0.60	lb			0.60	kg	
PM 2.5	0.0093	lb			0.0093	kg	
Sulfur Oxides	0.059	lb			0.059	kg	
Solid Wastes							
Landfilled	0.28	lb			0.28	kg	
Burned	3.62	lb			3.62	kg	
Waste-to-Energy	0.023	lb			0.023	kg	
Waterborne Wastes							
Acetone	1.0E-08	lb	(4)		1.0E-08	kg	
Benzene	1.0E-05	lb	(4)		1.0E-05	kg	
BOD	6.7E-04	lb			6.7E-04	kg	
COD	0.010	lb	(4)		0.010	kg	
Ethylbenzene	1.0E-05	lb	(4)		1.0E-05	kg	
Naphthalene	1.0E-08	lb	(4)		1.0E-08	kg	
Phenol	0.0010	lb	(4)		0.0010	kg	
Styrene	1.0E-06	lb	(4)		1.0E-06	kg	
Suspended Solids	0.0045	lb			0.0045	kg	
Toluene	1.0E-04	lb	(4)		1.0E-04	kg	
Total Organic Carbon	0.0010	lb	(4)		0.0010	kg	
Xylene	1.0E-06	lb	(4)		1.0E-06	kg	

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(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

(3) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(4) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(5) These fuel-related emissions were provided by the plants. These take into account the combustion of the off gas, as well as the natural gas.

References: B-34, B-35, B-39, B-40, and B-41.

Source: Franklin Associates, A Division of ERG

High-density Polyethylene Resin Production

High-density polyethylene is produced through the polymerization of ethylene. Polyethylene is manufactured by a slurry, solution, or a gas phase process. The average dataset includes data for the slurry and gas phase processes, which are discussed here. Ethylene and small amounts of co-monomers are continuously fed with a catalyst into a reactor.

In the slurry process, ethylene and co-monomers come into contact with the catalyst, which is suspended in a diluent. Particulates of polyethylene are then formed. After the diluent is removed, the reactor fluff is dried and pelletized.

In the gas phase process, a transition metal catalyst is introduced into a reactor containing ethylene gas, co-monomer, and a molecular control agent. The ethylene and co-monomer react to produce a polyethylene powder. The ethylene gas is separated from the powder, which is then pelletized.

A weighted average using production amounts was calculated from the HDPE production data from five plants collected from three leading producers in North America. The energy requirements and emissions data for the production of HDPE resin is displayed in Table B-7. Scrap is produced as a coproduct during this process. A mass basis was used to partition the credit for each product.

As of 2003, there were 10 HDPE producers and 23 HDPE plants in the U.S. (Reference B-43). While data was collected from a small sample of plants, the HDPE producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American HDPE production. The average dataset was reviewed and accepted by all HDPE data providers.

To assess the quality of the data collected for HDPE, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for HDPE include direct measurements, calculations from equipment specifications, information provided by purchasing and utility records, and estimates. The technology represented by the HDPE data represents a combination of UNIPOL gas and slurry processes. All data submitted for HDPE represent the year 2003 and U.S. and Canadian production.

Table B-7

DATA FOR THE PRODUCTION OF HIGH-DENSITY POLYETHYLENE (HDPE) RESIN

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Olefins	990	lb			990	kg	
Water Consumption	179	gal			1,494	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	80.7	kwh		858	178	kwh	2.00
Electricity (cogeneration)	662	cu ft	(1)	741	41.3	cu meters	1.73
Natural gas	569	cu ft		637	35.5	cu meters	1.48
LPG	0.0045	gal		0.49	0.038	liter	0.0011
Residual oil	0.72	gal		124	6.01	liter	0.29
Total Process				2,361			5.50
Environmental Emissions							
Atmospheric Emissions							
Carbon Monoxide	0.16	lb			0.16	kg	
Methane	0.014	lb			0.014	kg	
Nitrogen Oxides	0.029	lb			0.029	kg	
Hydrocarbons (NM)	0.42	lb			0.42	kg	
Other Organics	0.010	lb	(2)		0.010	kg	
Particulates (unknown)	0.018	lb			0.018	kg	
PM2.5	0.012	lb			0.012	kg	
PM10	0.041	lb			0.041	kg	
Sulfur Oxides	4.8E-05	lb			4.8E-05	kg	
Solid Wastes							
Landfilled	0.36	lb			0.36	kg	
Burned	0.26	lb			0.26	kg	
Waste-to-Energy	0.0040	lb			0.0040	kg	
Waterborne Wastes							
Aluminum	0.0010	lb	(2)		0.0010	kg	
BOD	0.0056	lb			0.0056	kg	
COD	0.0010	lb	(2)		0.0010	kg	
Chlorides	1.0E-06	lb	(2)		1.0E-06	kg	
Chromium	1.0E-05	lb	(2)		1.0E-05	kg	
Dissolved solids	0.044	lb			0.044	kg	
Furans	1.0E-06	lb	(2)		1.0E-06	kg	
Hydrocarbons	0.0010	lb	(2)		0.0010	kg	
Oil	0.0043	lb			0.0043	kg	
Phenol/Phenolics	1.0E-05	lb	(2)		1.0E-05	kg	
Phosphorus	1.0E-04	lb	(2)		1.0E-04	kg	
Process solvents	1.0E-04	lb	(2)		1.0E-04	kg	
Suspended solids	0.052	lb			0.052	kg	
Zinc	8.5E-05	lb			8.5E-05	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

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Source: Franklin Associates, A Division of ERG

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APPENDIX C

LOW-DENSITY POLYETHYLENE

INTRODUCTION

This appendix discusses the manufacture of low-density polyethylene (LDPE) resin. LDPE is commonly used to manufacture packaging films and extrusion coatings. Approximately 8 billion pounds of LDPE was produced in the U.S. and Canada in 2003 (Reference C-1). The material flow for LDPE resin is shown in Figure C-1. The total unit process energy and emissions data (cradle-to-LDPE) for LDPE are displayed in Table C-1. An individual process table on the bases of 1,000 pounds and 1,000 kilograms is shown within this appendix. Processes that have been discussed in the previous appendix have been omitted from this appendix. The following process is included in this appendix:

- LDPE resin production

Crude oil production, distillation, desalting, and hydrotreating, natural gas production, natural gas processing, and ethylene production are discussed in Appendix B.

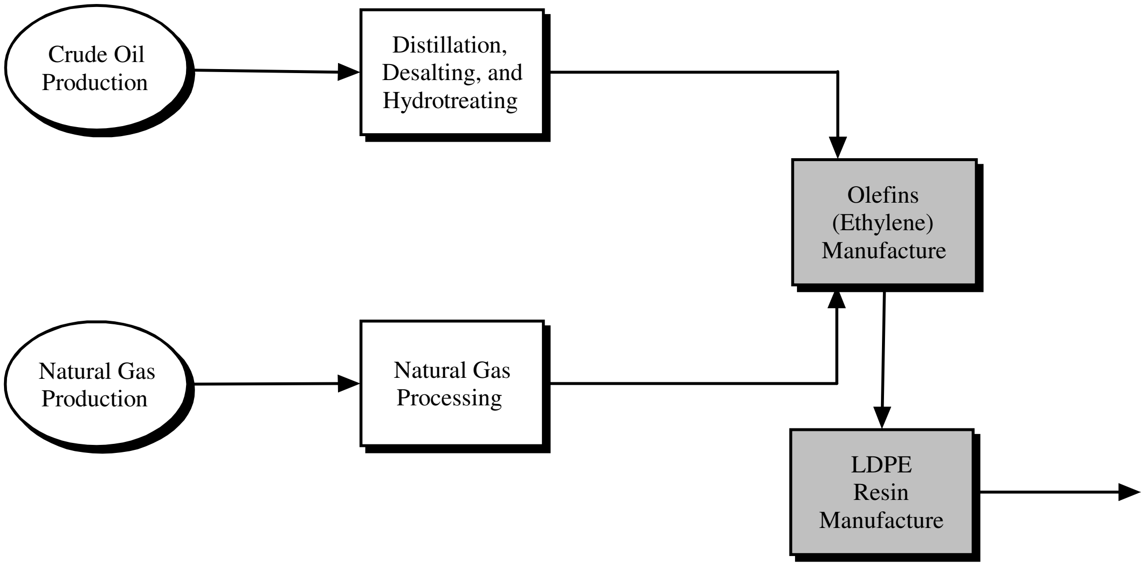

Figure C-1. Flow diagram for the manufacture of virgin low-density polyethylene (LDPE) resin. Shaded boxes represent partial or complete data provided by manufacturers specifically for this APC analysis.

Table C-1

DATA FOR THE PRODUCTION
OF LOW-DENSITY POLYETHYLENE (LDPE) RESIN
(Cradle-to-Resin)
(page 1 of 3)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	191	lb		191	kg	
Natural Gas	842	lb		842	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			18,023			42.0
Petroleum			3,584			8.34
Total Resource			21,607			50.3
Process Energy						
Electricity (grid)	166	kwh	1,761	365	kwh	4.10
Electricity (cogeneration)	2,376	cu ft (2)	2,661	148	cu meters	6.19
Natural gas	4,253	cu ft	4,763	265	cu meters	11.1
LPG	0.034	gal	3.65	0.28	liter	0.0085
Distillate oil	0.18	gal	29.0	1.52	liter	0.068
Residual oil	0.98	gal	168	8.15	liter	0.39
Gasoline	0.11	gal	16.1	0.94	liter	0.037
Diesel	0.0096	gal	1.52	0.080	liter	0.0035
Internal Offgas use (1)						
From Oil	26.3	lb	807	26.3	kg	1.88
From Natural Gas	120	lb	3,674	120	kg	8.55
Recovered Energy	183	thousand Btu	183	426	MJ	0.43
Total Process			13,700			31.9
Transportation Energy						
Combination truck	7.69	ton-miles		24.8	tonne-km	
Diesel	0.081	gal	12.8	0.67	liter	0.030
Rail	6.65	ton-miles		21.4	tonne-km	
Diesel	0.016	gal	2.62	0.14	liter	0.0061
Barge	15.8	ton-miles		51.0	tonne-km	
Diesel	0.013	gal	2.01	0.11	liter	0.0047
Residual oil	0.042	gal	7.23	0.35	liter	0.017
Ocean freighter	321	ton-miles		1,031	tonne-km	
Diesel	0.067	gal	10.7	0.56	liter	0.025
Residual	0.57	gal	98.3	4.78	liter	0.23
Pipeline-natural gas	478	ton-miles		1,540	tonne-km	
Natural gas	330	cu ft	370	20.6	cu meter	0.86
Pipeline-petroleum products	126	ton-miles		406	tonne-km	
Electricity	2.75	kwh	29.2	6.06	kwh	0.068
Total Transportation			533			1.24

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table C-1

DATA FOR THE PRODUCTION
OF LOW-DENSITY POLYETHYLENE (LDPE) RESIN
(Cradle-to-Resin)
(page 2 of 3)

	English units (Basis: 1,000 lb)		**SI units (Basis: 1,000 kg)**	
Environmental Emissions				
Atmospheric Emissions				
Ammonia	7.7E-04	lb	7.7E-04	kg
Antimony	4.4E-07	lb	4.4E-07	kg
Arsenic	5.5E-08	lb	5.5E-08	kg
Benzene	0.093	lb	0.093	kg
Carbon Dioxide - Fossil	77.4		77.4	kg
Carbon Monoxide	0.10	lb	0.10	kg
Carbon Tetrachloride	2.9E-07	lb	2.9E-07	kg
CFC 13 (Methane, trichlorofluoro-)	4.7E-06	lb	4.7E-06	kg
Chlorine	1.0E-04	lb	1.0E-04	kg
Chromium	1.4E-07	lb	1.4E-07	kg
Ethylbenzene	0.011	lb	0.011	kg
Ethylene Dibromide	9.1E-07	lb	9.1E-07	kg
HCFC-22	0.0010	lb	0.0010	kg
Hydrogen	0.0040	lb	0.0040	kg
Hydrogen Chloride	1.0E-06	lb	1.0E-06	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.15	lb	0.15	kg
Methane	6.24	lb	6.24	kg
Nickel	1.2E-06	lb	1.2E-06	kg
Nitrogen Oxides	0.092	lb	0.092	kg
Nitrous Oxide	0.0010	lb	0.0010	kg
Non-Methane Hydrocarbons	0.96	lb	0.96	kg
Other Organics	0.051	lb	0.051	kg
Particulates (PM10)	0.13	lb	0.13	kg
Particulates (PM2.5)	0.010	lb	0.010	kg
Particulates (unspecified)	0.054	lb	0.054	kg
Polyaromatic Hydrocarbons (total)	1.2E-05	lb	1.2E-05	kg
Sulfur Dioxide	1.87	lb	1.87	kg
Sulfur Oxides	0.0042	lb	0.0042	kg
Toluene	0.14	lb	0.14	kg
VOC	0.75	lb	0.75	kg
Xylene	0.083	lb	0.083	kg
Solid Wastes				
Landfilled	32.3	lb	32.3	kg
Burned	3.89	lb	3.89	kg
Waste-to-Energy	0.024	lb	0.024	kg
Waterborne Wastes				
m-Xylene	8.6E-06	lb	8.6E-06	kg
1-Methylfluorene	2.0E-08	lb	2.0E-08	kg
2,4-Dimethylphenol	8.2E-06	lb	8.2E-06	kg
2-Hexanone	1.9E-06	lb	1.9E-06	kg
2-Methylnaphthalene	4.5E-06	lb	4.5E-06	kg
4-Methyl-2-Pentanone	7.5E-07	lb	7.5E-07	kg
Acetone	1.8E-06	lb	1.8E-06	kg
Acid (benzoic)	3.0E-04	lb	3.0E-04	kg
Acid (hexanoic)	6.2E-05	lb	6.2E-05	kg
Alkylated benzenes	5.5E-05	lb	5.5E-05	kg
Alkylated fluorenes	3.2E-06	lb	3.2E-06	kg
Alkylated naphthalenes	9.0E-07	lb	9.0E-07	kg
Alkylated phenanthrenes	3.7E-07	lb	3.7E-07	kg
Aluminum	0.027	lb	0.027	kg
Ammonia	0.0063	lb	0.0063	kg
Antimony	1.7E-05	lb	1.7E-05	kg
Arsenic	5.5E-05	lb	5.5E-05	kg
Barium	0.36	lb	0.36	kg
Benzene	3.2E-04	lb	3.2E-04	kg
Beryllium	3.5E-06	lb	3.5E-06	kg
BOD	0.047	lb	0.047	kg
Boron	9.2E-04	lb	9.2E-04	kg
Bromide	0.036	lb	0.036	kg
Cadmium	8.6E-06	lb	8.6E-06	kg
Calcium	0.59	lb	0.59	kg
CFC-11	1.0E-04	lb	1.0E-04	kg
Chlorides	7.38	lb	7.38	kg
Chromium (unspecified)	7.2E-04	lb	7.2E-04	kg
Cobalt	6.5E-06	lb	6.5E-06	kg
COD	0.21	lb	0.21	kg
Copper	7.8E-05	lb	7.8E-05	kg

Table C-1

DATA FOR THE PRODUCTION
OF LOW-DENSITY POLYETHYLENE (LDPE) RESIN
(Cradle-to-Resin)
(page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Cyanide	1.3E-08	lb	1.3E-08	kg
Dibenzofuran	3.4E-08	lb	3.4E-08	kg
Dibenzothiophene	2.8E-08	lb	2.8E-08	kg
Dissolved Solids	7.40	lb	7.40	kg
Ethylbenzene	2.7E-05	lb	2.7E-05	kg
Fluorene	1.5E-06	lb	1.5E-06	kg
Iron	0.050	lb	0.050	kg
Isopropyl alcohol	1.0E-04	lb	1.0E-04	kg
Lead	1.5E-04	lb	1.5E-04	kg
Lead 210	3.0E-14	lb	3.0E-14	kg
Lithium	0.14	lb	0.14	kg
Magnesium	0.12	lb	0.12	kg
Manganese	1.7E-04	lb	1.7E-04	kg
Mercury	3.1E-07	lb	3.1E-07	kg
Methyl Chloride	7.2E-09	lb	7.2E-09	kg
Methyl Ethyl Ketone	1.4E-08	lb	1.4E-08	kg
Molybdenum	6.7E-06	lb	6.7E-06	kg
Naphthalene	5.3E-06	lb	5.3E-06	kg
n-Decane	8.5E-06	lb	8.5E-06	kg
n-Docosane	1.9E-07	lb	1.9E-07	kg
n-Dodecane	1.6E-05	lb	1.6E-05	kg
n-Eicosane	4.4E-06	lb	4.4E-06	kg
n-Hexacosane	1.2E-07	lb	1.2E-07	kg
n-Hexadecane	1.8E-05	lb	1.8E-05	kg
Nickel	6.7E-05	lb	6.7E-05	kg
n-Octadecane	4.4E-06	lb	4.4E-06	kg
p -Xylene	3.2E-06	lb	3.2E-06	kg
o -Xylene	3.2E-06	lb	3.2E-06	kg
o-Cresol	8.4E-06	lb	8.4E-06	kg
Oil	0.0085	lb	0.0085	kg
p-Cresol	9.1E-06	lb	9.1E-06	kg
p-Cymene	1.8E-08	lb	1.8E-08	kg
Pentamethylbenzene	1.3E-08	lb	1.3E-08	kg
Phenanthrene	2.3E-07	lb	2.3E-07	kg
Phenol/ Phenolic Compounds	0.0011	lb	0.0011	kg
Phosphorus	1.0E-04	lb	1.0E-04	kg
Tetradecane	6.9E-06	lb	6.9E-06	kg
Radium 226	1.1E-11	lb	1.1E-11	kg
Radium 228	5.4E-14	lb	5.4E-14	kg
Selenium	3.6E-06	lb	3.6E-06	kg
Silver	3.6E-04	lb	3.6E-04	kg
Sodium	1.69	lb	1.69	kg
Strontium	0.016	lb	0.016	kg
Styrene	1.0E-06	lb	1.0E-06	kg
Sulfates	0.012	lb	0.012	kg
Sulfides	4.0E-05	lb	4.0E-05	kg
Sulfur	7.4E-04	lb	7.4E-04	kg
Surfactants	1.5E-04	lb	1.5E-04	kg
Suspended Solids	2.99	lb	2.99	kg
Thallium	3.5E-06	lb	3.5E-06	kg
Tin	6.7E-05	lb	6.7E-05	kg
Titanium	2.6E-04	lb	2.6E-04	kg
TOC	0.0010	lb	0.0010	kg
Toluene	3.8E-04	lb	3.8E-04	kg
Total biphenyls	3.5E-06	lb	3.5E-06	kg
Total dibenzothiophenes	1.1E-08	lb	1.1E-08	kg
Vanadium	1.9E-05	lb	1.9E-05	kg
Xylene, unspecified	1.3E-04	lb	1.3E-04	kg
Yttrium	2.0E-06	lb	2.0E-06	kg
Zinc	6.2E-04	lb	6.2E-04	kg

References: Tables B-2 through B-6 and C-2.

Source: Franklin Associates, A Division of ERG models

LDPE Resin Production

Low-density polyethylene (LDPE) is produced by the polymerization of ethylene in high pressure reactors (above 3,000 psi). This is the standard technology for LDPE production. The two reactor types used are autoclaves and tubular reactors. Generally, tubular reactors operate at a higher average ethylene conversion than autoclave reactors. The polymerization mechanism is either free-radical, using peroxide initiators, or ionic polymerization, using Ziegler catalyst.

Reactor effluent consists of unreacted ethylene and polymer. The pressure of the effluent mixture is reduced and the ethylene is purified and recycled back to the reactor.

A weighted average using production amounts was calculated from the LDPE production data from seven plants collected from three leading producers in North America. Table C-2 displays the energy and emissions data for the production of LDPE resin. Scrap and steam are produced as coproducts during this process. A mass basis was used to partition the credit for scrap, while the energy amount for the steam was reported separately as recovered energy.

As of 2003, there were 8 LDPE producers and 15 LDPE plants in the U.S. (Reference C-3). The LDPE data collected for this module represents a majority of North American LDPE production. The average dataset was reviewed and accepted by all LDPE data providers.

To assess the quality of the data collected for LDPE, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for LDPE include direct measurements, information provided by purchasing and utility records, and estimates. The technology represented by the LDPE data represents a combination of the tubular and autoclave high-pressure reactors. All data submitted for LDPE represent the years 2002 and 2003 and production in U.S. and Canada.

Table C-2

DATA FOR THE PRODUCTION OF LOW-DENSITY POLYETHYLENE (LDPE) RESIN

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Olefins	1,008	lb			1,008	kg	
Water Consumption	499	gal			4,164	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	85.5	kwh		909	188	kwh	2.12
Electricity (cogeneration)	2,172	cu ft	(1)	2,432	136	cu meters	5.66
Natural gas	775	cu ft		868	48.4	cu meters	2.02
LPG	0.0038	gal		0.41	0.032	liter	9.6E-04
Residual oil	0.16	gal		27.4	1.33	liter	0.064
Recovered Energy	171	thousand Btu		171	398	MJ	0.40
Total Process				4,066			9.47
Environmental Emissions							
Atmospheric Emissions							
Carbon Monoxide	0.010	lb	(2)		0.010	kg	
Carbon Dioxide	10.0	lb	(2)		10.0	kg	
Chlorine	1.0E-06	lb	(2)		1.0E-06	kg	
HCFC-22	0.0010	lb	(2)		0.0010	kg	
Methane	0.0066	lb			0.0066	kg	
NM Hydrocarbons	0.87	lb			0.87	kg	
Nitrogen Oxides	0.0010	lb	(2)		0.0010	kg	
Nitrous Oxide	0.0010	lb	(2)		0.0010	kg	
Other Organics	0.050	lb			0.050	kg	
Particulates (unknown)	0.045	lb			0.045	kg	
PM2.5	0.0055	lb			0.0055	kg	
PM10	0.026	lb			0.026	kg	
Sulfur Oxides	1.0E-05	lb	(2)		1.0E-05	kg	
Solid Wastes							
Landfilled	0.063	lb			0.063	kg	
Burned	0.24	lb			0.24	kg	
Waterborne Wastes							
Aluminum	1.0E-04	lb	(2)		1.0E-04	kg	
BOD	0.010	lb	(2)		0.010	kg	
COD	0.10	lb	(2)		0.10	kg	
Dissolved Solids	0.0010	lb	(2)		0.0010	kg	
CFC-011	1.0E-04	lb	(2)		1.0E-04	kg	
Isopropyl Alcohol	1.0E-04	lb	(2)		1.0E-04	kg	
Oil	0.0010	lb	(2)		0.0010	kg	
Phenol/Phenolics	1.0E-06	lb	(2)		1.0E-06	kg	
Phosphorus	1.0E-04	lb	(2)		1.0E-04	kg	
Suspended Solids	0.010	lb	(2)		0.010	kg	
Zinc	1.0E-05	lb	(2)		1.0E-05	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

References: C-2

Source: Franklin Associates, A Division of ERG

REFERENCES

C-1. APC Plastics Industry Producers' Statistics Group, as compiled by VERIS Consulting, LLC. 2004.

C-2. Information and data collected from APC member and non-member companies producing LDPE. 2004-2005.

C-3. Chemical profile information taken from the website: http://www.the-innovation-group.com/welcome.htm.

APPENDIX D

LINEAR LOW-DENSITY POLYETHYLENE

INTRODUCTION

This appendix discusses the manufacture of linear low-density polyethylene (LLDPE) resin. LLDPE is commonly used to manufacture shrink/stretch film and trash bags. More than 11 billion pounds of LDPE was produced in the U.S. and Canada in 2003 (Reference D-1). The material flow for LLDPE resin is shown in Figure D-1. The total unit process energy and emissions data (cradle-to-LLDPE) for LLDPE are displayed in Table D-1. An individual process table on the bases of 1,000 pounds and 1,000 kilograms is shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following process is included in this appendix:

- LLDPE resin production

Crude oil production, distillation, desalting, and hydrotreating, natural gas production, natural gas processing, and ethylene production are discussed in Appendix B.

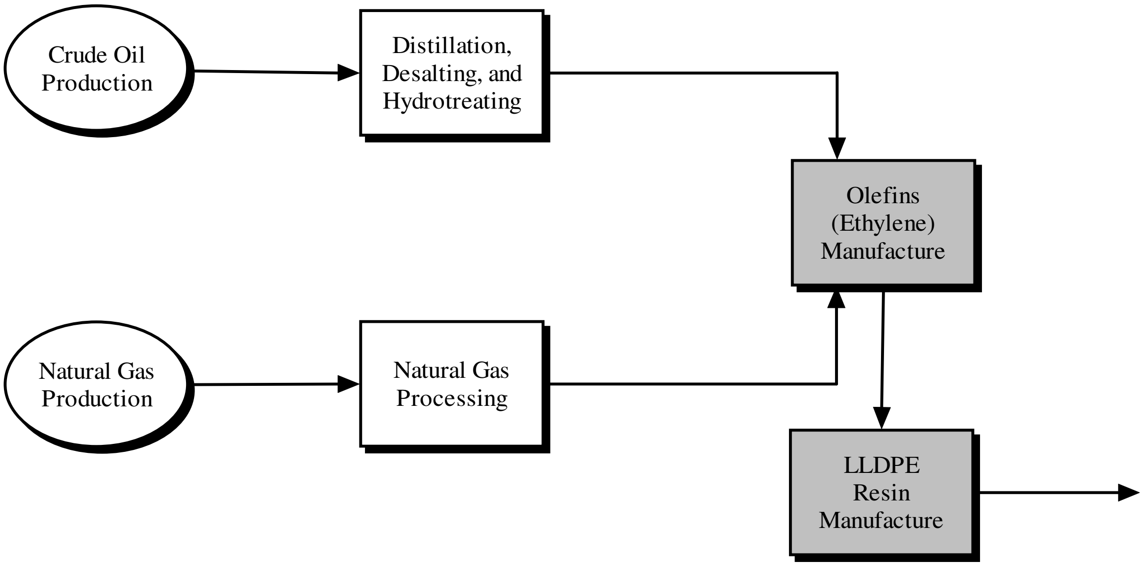

Figure D-1. Flow diagram for the manufacture of virgin linear low-density (LLDPE) resin. Shaded boxes represent partial or complete data provided by manufacturers specifically for this analysis.

Table D-1

DATA FOR THE PRODUCTION
OF LINEAR LOW-DENSITY POLYETHYLENE (LLDPE) RESIN
(Cradle-to-Resin)
(page 1 of 3)

	English units (Basis: 1,000 lb)			**SI units (Basis: 1,000 kg)**		
Raw Materials						
Crude oil	189	lb		189	kg	
Natural Gas	834	lb		834	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			17,867			41.6
Petroleum			3,554			8.27
Total Resource			21,421			49.9
Process Energy						
Electricity (grid)	137	kwh	1,457	302	kwh	3.39
Electricity (cogeneration)	661	cu ft (2)	740	41.3	cu meters	1.72
Natural gas	4,122	cu ft	4,617	257	cu meters	10.7
LPG	0.030	gal	3.21	0.25	liter	0.0075
Distillate oil	0.18	gal	28.8	1.51	liter	0.067
Residual oil	1.21	gal	207	10.1	liter	0.48
Gasoline	0.11	gal	16.1	0.95	liter	0.037
Diesel	0.010	gal	1.63	0.086	liter	0.0038
Internal Offgas use (1)						
From Oil	26.1	lb	800	26.1	kg	1.86
From Natural Gas	119	lb	3,642	119	kg	8.48
Recovered Energy	12.0	thousand Btu	12.0	27.9	MJ	0.028
Total Process			11,501			26.8
Transportation Energy						
Combination truck	7.63	ton-miles		24.5	tonne-km	
Diesel	0.080	gal	12.7	0.67	liter	0.030
Rail	6.59	ton-miles		21.2	tonne-km	
Diesel	0.016	gal	2.59	0.14	liter	0.0060
Barge	15.7	ton-miles		50.5	tonne-km	
Diesel	0.013	gal	2.00	0.10	liter	0.0046
Residual oil	0.042	gal	7.17	0.35	liter	0.017
Ocean freighter	318	ton-miles		1,023	tonne-km	
Diesel	0.067	gal	10.6	0.56	liter	0.025
Residual	0.54	gal	93.2	4.53	liter	0.22
Pipeline-natural gas	474	ton-miles		1,527	tonne-km	
Natural gas	327	cu ft	367	20.4	cu meter	0.85
Pipeline-petroleum products	125	ton-miles		402	tonne-km	
Electricity	2.72	kwh	27.9	6.01	kwh	0.065
Total Transportation			523			1.22

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table D-1

DATA FOR THE PRODUCTION
OF LINEAR LOW-DENSITY POLYETHYLENE (LLDPE) RESIN
(Cradle-to-Resin)
(page 2 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Aluminum Compounds	1.0E-04	lb	1.0E-04	kg
Ammonia	7.6E-04	lb	7.6E-04	kg
Antimony	4.3E-07	lb	4.3E-07	kg
Arsenic	5.5E-08	lb	5.5E-08	kg
Benzene	0.092	lb	0.092	kg
Carbon Dioxide - Fossil	118	lb	118	kg
Carbon Monoxide	0.19	lb	0.19	kg
Carbon Tetrachloride	2.9E-07	lb	2.9E-07	kg
CFC 13 (Methane, trichlorofluoro-)	4.6E-06	lb	4.6E-06	kg
Chlorine	1.0E-04	lb	1.0E-04	kg
Chromium	1.4E-07	lb	1.4E-07	kg
Ethylbenzene	0.011	lb	0.011	kg
Ethylene Dibromide	9.1E-07	lb	9.1E-07	kg
Furans	0.0010	lb	0.0010	kg
HCFC-22	1.1E-05	lb	1.1E-05	kg
Hydrogen	0.0039	lb	0.0039	kg
Hydrogen Chloride	1.0E-06	lb	1.0E-06	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.14	lb	0.14	kg
Methane	6.18	lb	6.18	kg
Nickel	1.2E-06	lb	1.2E-06	kg
Nitrogen Oxides	0.12	lb	0.12	kg
Nitrous Oxide	0.017	lb	0.017	kg
Non-Methane Hydrocarbons	0.45	lb	0.45	kg
Other Organics	0.011	lb	0.011	kg
Particulates (PM10)	0.12	lb	0.12	kg
Particulates (PM2.5)	0.015	lb	0.015	kg
Particulates (unspecified)	0.018	lb	0.018	kg
Polyaromatic Hydrocarbons (total)	1.2E-05	lb	1.2E-05	kg
Sulfur Dioxide	1.85	lb	1.85	kg
Sulfur Oxides	0.0043	lb	0.0043	kg
Toluene	0.14	lb	0.14	kg
VOC	0.74	lb	0.74	kg
Xylene	0.082	lb	0.082	kg
Solid Wastes				
Landfilled	32.3	lb	32.3	kg
Burned	3.75	lb	3.75	kg
Waste-to-Energy	0.11	lb	0.11	kg
Waterborne Wastes				
m-Xylene	8.5E-06	lb	8.5E-06	kg
1-Methylfluorene	2.0E-08	lb	2.0E-08	kg
2,4-Dimethylphenol	8.1E-06	lb	8.1E-06	kg
2-Hexanone	1.9E-06	lb	1.9E-06	kg
2-Methylnaphthalene	4.5E-06	lb	4.5E-06	kg
4-Methyl-2-Pentanone	7.4E-07	lb	7.4E-07	kg
Acetone	1.8E-06	lb	1.8E-06	kg
Acid (benzoic)	2.9E-04	lb	2.9E-04	kg
Acid (hexanoic)	6.1E-05	lb	6.1E-05	kg
Alkylated benzenes	5.4E-05	lb	5.4E-05	kg
Alkylated fluorenes	3.1E-06	lb	3.1E-06	kg
Alkylated naphthalenes	8.9E-07	lb	8.9E-07	kg
Alkylated phenanthrenes	3.7E-07	lb	3.7E-07	kg
Aluminum	0.028	lb	0.028	kg
Ammonia	0.0062	lb	0.0062	kg
Antimony	1.7E-05	lb	1.7E-05	kg
Arsenic	5.5E-05	lb	5.5E-05	kg
Barium	0.36	lb	0.36	kg
Benzene	3.2E-04	lb	3.2E-04	kg
Beryllium	3.5E-06	lb	3.5E-06	kg
BOD	0.038	lb	0.038	kg
Boron	9.1E-04	lb	9.1E-04	kg
Bromide	0.035	lb	0.035	kg
Butene	1.0E-04	lb	1.0E-04	kg
Cadmium	8.5E-06	lb	8.5E-06	kg
Calcium	0.59	lb	0.59	kg
Chlorides	7.32	lb	7.32	kg
Chromium (unspecified)	7.1E-04	lb	7.1E-04	kg

Table D-1

DATA FOR THE PRODUCTION
OF LINEAR LOW-DENSITY POLYETHYLENE (LLDPE) RESIN
(Cradle-to-Resin)
(page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Cobalt	6.4E-06	lb	6.4E-06	kg
COD	0.12	lb	0.12	kg
Copper	7.7E-05	lb	7.7E-05	kg
Cyanide	1.3E-08	lb	1.3E-08	kg
Cyclohexane	1.0E-04	lb	1.0E-04	kg
Dibenzofuran	3.4E-08	lb	3.4E-08	kg
Dibenzothiophene	2.7E-08	lb	2.7E-08	kg
Dissolved Solids	7.36	lb	7.36	kg
Ethylbenzene	2.7E-05	lb	2.7E-05	kg
Fluorene	1.5E-06	lb	1.5E-06	kg
Iron	0.049	lb	0.049	kg
Lead	1.5E-04	lb	1.5E-04	kg
Lead 210	3.0E-14	lb	3.0E-14	kg
Lithium	0.14	lb	0.14	kg
Magnesium	0.12	lb	0.12	kg
Manganese	1.7E-04	lb	1.7E-04	kg
Mercury	3.0E-07	lb	3.0E-07	kg
Methyl Chloride	7.1E-09	lb	7.1E-09	kg
Methyl Ethyl Ketone	1.4E-08	lb	1.4E-08	kg
Molybdenum	6.7E-06	lb	6.7E-06	kg
Naphthalene	5.3E-06	lb	5.3E-06	kg
n-Decane	8.4E-06	lb	8.4E-06	kg
n-Docosane	1.9E-07	lb	1.9E-07	kg
n-Dodecane	1.6E-05	lb	1.6E-05	kg
n-Eicosane	4.4E-06	lb	4.4E-06	kg
n-Hexacosane	1.2E-07	lb	1.2E-07	kg
n-Hexadecane	1.7E-05	lb	1.7E-05	kg
Nickel	6.7E-05	lb	6.7E-05	kg
n-Octadecane	4.3E-06	lb	4.3E-06	kg
p -Xyxlene	3.1E-06	lb	3.1E-06	kg
o -Xyxlene	3.1E-06	lb	3.1E-06	kg
o-Cresol	8.4E-06	lb	8.4E-06	kg
Oil	0.011	lb	0.011	kg
p-Cresol	9.0E-06	lb	9.0E-06	kg
p-Cymene	1.8E-08	lb	1.8E-08	kg
Pentamethylbenzene	1.3E-08	lb	1.3E-08	kg
Phenanthrene	2.3E-07	lb	2.3E-07	kg
Phenol/ Phenolic Compounds	0.0011	lb	0.0011	kg
Phosphorus	1.0E-04	lb	1.0E-04	kg
Process solvents	1.0E-04	lb	1.0E-04	kg
Tetradecane	6.9E-06	lb	6.9E-06	kg
Radium 226	1.1E-11	lb	1.1E-11	kg
Radium 228	5.4E-14	lb	5.4E-14	kg
Selenium	3.6E-06	lb	3.6E-06	kg
Silver	3.6E-04	lb	3.6E-04	kg
Sodium	1.68	lb	1.68	kg
Strontium	0.016	lb	0.016	kg
Styrene	1.0E-06	lb	1.0E-06	kg
Sulfates	0.012	lb	0.012	kg
Sulfides	4.0E-05	lb	4.0E-05	kg
Sulfur	7.3E-04	lb	7.3E-04	kg
Surfactants	1.4E-04	lb	1.4E-04	kg
Suspended Solids	2.98	lb	2.98	kg
Thallium	3.5E-06	lb	3.5E-06	kg
Tin	6.6E-05	lb	6.6E-05	kg
Titanium	2.6E-04	lb	2.6E-04	kg
TOC	0.0010	lb	0.0010	kg
Toluene	3.8E-04	lb	3.8E-04	kg
Total biphenyls	3.5E-06	lb	3.5E-06	kg
Total dibenzothiophenes	1.1E-08	lb	1.1E-08	kg
Vanadium	1.9E-05	lb	1.9E-05	kg
Xylene, unspecified	1.3E-04	lb	1.3E-04	kg
Yttrium	2.0E-06	lb	2.0E-06	kg
Zinc	6.1E-04	lb	6.1E-04	kg

References: Tables B-2 through B-6 and D-2.

Source: Franklin Associates, A Division of ERG models

LLDPE Resin Production

LLDPE is produced through the polymerization of ethylene. Polyethylene is most commonly manufactured by either a solution process or a gas phase process. The data in this module represent solution and gas phase technologies. Ethylene and small amounts of co-monomers are continuously fed with a catalyst into a reactor.

In the solution process, ethylene and co-monomers come into contact with the catalyst, which is suspended in a diluent. Particulates of polyethylene are then formed. After the diluent is removed, the reactor fluff is dried and pelletized.

In the gas phase process, a transition metal catalyst is introduced into a reactor containing ethylene gas, co-monomer, and a molecular control agent. The ethylene and co-monomer react to produce a polyethylene powder. The ethylene gas is separated from the powder, which is then pelletized.

A weighted average using production amounts was calculated from the LLDPE production data from five plants collected from three leading producers in North America. Table D-2 displays the energy and emissions data for the production of LLDPE resin. Scrap is produced as a coproduct during this process. A mass basis was used to partition the credit for scrap.

As of 2003, there were 11 LLDPE producers and 24 LLDPE plants in the U.S. (Reference D-3). While data was collected from a small sample of plants, the LLDPE producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American LLDPE production. The average dataset was reviewed and accepted by all LLDPE data providers.

To assess the quality of the data collected for LLDPE, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for LLDPE include direct measurements, information provided by purchasing and utility records, and estimates. The technology represented by the LLDPE data represents a combination of the solution and gas phase processes. All data submitted for LLDPE represent the year 2003 and production in U.S. and Canada.

Table D-2

DATA FOR THE PRODUCTION OF LINEAR LOW-DENSITY POLYETHYLENE (LLDPE) RESIN

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Olefins	999	lb			999	kg	
Water Consumption	60.0	gal			501	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	57.6	kwh		613	127	kwh	1.43
Electricity (cogeneration)	459	cu ft	(1)	514	28.6	cu meters	1.20
Natural gas	674	cu ft		755	42.1	cu meters	1.76
Residual oil	0.40	gal		68.6	3.34	liter	0.16
Gasoline	0.0010	gal		0.14	0.0083	liter	3.3E-04
Diesel	7.5E-04	gal		0.12	0.0063	liter	2.8E-04
Total Process				1,950			4.54
Environmental Emissions							
Atmospheric Emissions							
Aluminum Compounds	1.0E-04	lb	(2)		1.0E-04	kg	
Carbon Dioxide (fossil)	50.8	lb			50.8	kg	
Carbon Monoxide	0.10	lb			0.10	kg	
Furans	0.0010	lb	(2)		0.0010	kg	
HCFC-22	1.0E-05	lb	(2)		1.0E-05	kg	
Methane	0.0020	lb			0.0020	kg	
Nitrogen Oxides	0.030	lb			0.030	kg	
Nitrous Oxides	0.017	lb			0.017	kg	
NM Hydrocarbons	0.36	lb			0.36	kg	
Other Organics	0.010	lb	(2)		0.010	kg	
Particulates (unknown)	0.010	lb	(2)		0.010	kg	
PM2.5	0.010	lb	(2)		0.010	kg	
PM10	0.014	lb			0.014	kg	
Sulfur Oxides	1.6E-04	lb			1.6E-04	kg	
Solid Wastes							
Landfilled	0.35	lb			0.35	kg	
Burned	0.13	lb			0.13	kg	
Waste-to-Energy	0.091	lb			0.091	kg	
Waterborne Wastes							
Aluminum	0.0010	lb	(2)		0.0010	kg	
BOD	0.0010	lb	(2)		0.0010	kg	
Butene	1.0E-04	lb	(2)		1.0E-04	kg	
COD	0.010	lb	(2)		0.010	kg	
Cyclohexane	1.0E-04	lb	(2)		1.0E-04	kg	
Dissolved Solids	0.024	lb			0.024	kg	
Oil & Grease	0.0034	lb			0.0034	kg	
Phenolics	1.0E-06	lb	(2)		1.0E-06	kg	
Phosphorus	1.0E-04	lb	(2)		1.0E-04	kg	
Process Solvents	1.0E-04	lb	(2)		1.0E-04	kg	
Suspended Solids	0.034	lb			0.034	kg	
Zinc	1.0E-05	lb	(2)		1.0E-05	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

References: D-2

Source: Franklin Associates, A Division of ERG

REFERENCES

D-1. APC Plastics Industry Producers' Statistics Group, as compiled by VERIS Consulting, LLC. 2004.

D-2. Information and data collected from APC member and non-member companies producing LLDPE. 2004-2005.

D-3. Chemical profile information taken from the website: http://www.the-innovation-group.com/welcome.htm.

APPENDIX E

POLYPROPYLENE

INTRODUCTION

This appendix discusses the manufacture of polypropylene (PP) resin. PP is used to manufacture textiles, rigid packaging, and consumer products. More than 17 billion pounds of PP was produced in the U.S. and Canada in 2003 (Reference E-1). The material flow for PP resin is shown in Figure E-1. The total unit process energy and emissions data (cradle-to-PP) for PP are displayed in Table E-1. An individual process table on the bases of 1,000 pounds and 1,000 kilograms is shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following process is included in this appendix:

- Propylene production
- Polypropylene resin production

Crude oil production, distillation, desalting, and hydrotreating, natural gas production, and natural gas processing are discussed in Appendix B.

Olefins Production (Propylene)

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

Typical production of ethylene, propylene, and other coproducts begins when hydrocarbons and steam are fed to the cracking furnace. After being heated to temperatures around 1,000° Celsius, the cracked products are quenched in heat exchangers which produce high pressure steam. Fuel oil is separated from the main gas stream in a multi-stage centrifugal compressor. The main gas stream then undergoes hydrogen sulfide removal and drying. The final step involves fractional distillation of the various reaction products.

Within the hydrocracker, an offgas is produced from the raw materials entering. A portion of this offgas is used within the hydrocracker to produce steam, while the remaining portion is exported from the hydrocracker as a coproduct, as discussed below. The offgas used within the hydrocracker is shown in Table E-2 as “Internal offgas use.” This offgas is shown as a weight of natural gas and petroleum input to produce the energy, as well as the energy amount produced from those weights.

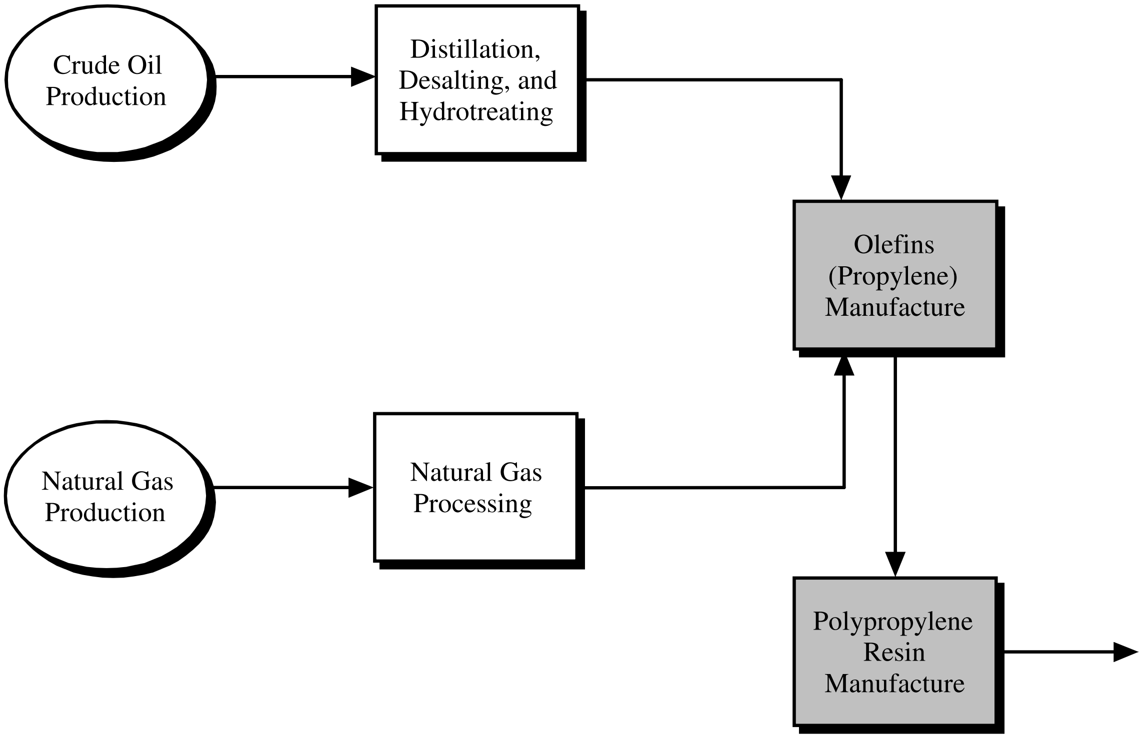

Figure E-1. Flow diagram for the manufacture of virgin polypropylene (PP) resin. Shaded boxes represent partial or complete data provided by manufacturers specifically for this APC analysis.

Data was collected from individual plants, and a mass allocation was used to provide an output of 1,000 pounds/kilograms of olefin product. Then a weighted average using propylene production amounts was applied to the individual olefins plant production data collected from three leading producers (8 thermal cracking units) in North America. Transportation amounts for propylene were calculated using a weighted average of data collected from the polypropylene producers. Numerous coproduct streams are produced during this process. Fuel gas and off-gas were two of the coproducts produced that were exported to another process for fuel use. When these fuel coproducts are exported from the hydrocracker, they carry with them the allocated share of the inputs and outputs for their production. The ratio of the mass of the exported fuel over the total mass output was removed from the total inputs and outputs of the hydrocracker, and the remaining inputs and outputs are allocated over the material hydrocracker products (Equation 1).

Table E-1

DATA FOR THE PRODUCTION
OF POLYPROPYLENE (PP) RESIN
(Cradle-to-Resin)
(page 1 of 3)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	367	lb		367	kg	
Natural Gas	644	lb		644	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			13,788			32.1
Petroleum			6,890			16.0
Total Resource			20,678			48.1
Process Energy						
Electricity (grid)	176	kwh	1,874	388	kwh	4.36
Electricity (cogeneration)	594	cu ft (2)	665	37.1	cu meters	1.55
Natural gas	3,185	cu ft	3,568	199	cu meters	8.31
LPG	0.060	gal	6.46	0.50	liter	0.015
Distillate oil	0.18	gal	29.2	1.53	liter	0.068
Residual oil	2.03	gal	348	16.9	liter	0.81
Gasoline	0.10	gal	14.9	0.87	liter	0.035
Diesel	0.0018	gal	0.28	0.015	liter	6.6E-04
Internal Offgas use (1)						
From Oil	66.0	lb	1,877	66.0	kg	4.37
From Natural Gas	117	lb	3,336	117	kg	7.77
Recovered Energy	2.29	thousand Btu	2.29	5.33	MJ	0.0053
Total Process			11,717			27.3
Transportation Energy						
Combination truck	9.59	ton-miles		30.9	tonne-km	
Diesel	0.10	gal	16.0	0.84	liter	0.037
Rail	7.50	ton-miles		24.1	tonne-km	
Diesel	0.019	gal	2.95	0.16	liter	0.0069
Barge	31.6	ton-miles		102	tonne-km	
Diesel	0.025	gal	4.01	0.21	liter	0.0093
Residual oil	0.084	gal	14.4	0.70	liter	0.034
Ocean freighter	639	ton-miles		2,057	tonne-km	
Diesel	0.12	gal	19.3	1.01	liter	0.045
Residual	1.09	gal	186	9.07	liter	0.43
Pipeline-natural gas	379	ton-miles		1,219	tonne-km	
Natural gas	261	cu ft	293	16.3	cu meter	0.68
Pipeline-petroleum products	150	ton-miles		483	tonne-km	
Electricity	3.27	kwh	33.5	7.22	kwh	0.078
Total Transportation			569			1.32

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table E-1

**DATA FOR THE PRODUCTION
OF POLYPROPYLENE (PP) RESIN
(Cradle-to-Resin)
(page 2 of 3)**

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Ammonia	0.0015	lb	0.0015	kg
Antimony	8.7E-07	lb	8.7E-07	kg
Arsenic	1.1E-07	lb	1.1E-07	kg
Benzene	0.074	lb	0.074	kg
Carbon Dioxide - Fossil	73.0	lb	73.0	kg
Carbon Monoxide	0.30	lb	0.30	kg
Carbon Tetrachloride	5.8E-07	lb	5.8E-07	kg
CFC 13 (Methane, trichlorofluoro-)	9.3E-06	lb	9.3E-06	kg
Chlorine	1.0E-04	lb	1.0E-04	kg
Chromium	2.9E-07	lb	2.9E-07	kg
Ethylbenzene	0.0087	lb	0.0087	kg
Ethylene Dibromide	1.8E-06	lb	1.8E-06	kg
HCFC-22	1.0E-06	lb	1.0E-06	kg
Hydrogen	0.0052	lb	0.0052	kg
Hydrogen Chloride	1.0E-06	lb	1.0E-06	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.29	lb	0.29	kg
Lead	1.0E-12	lb	1.0E-12	kg
Methane	6.40	lb	6.40	kg
Nickel	2.5E-06	lb	2.5E-06	kg
Nitrogen Oxides	0.19	lb	0.19	kg
Nitrous Oxide	0.0045	lb	0.0045	kg
Non-Methane Hydrocarbons	0.26	lb	0.26	kg
Other Organics	0.011	lb	0.011	kg
Particulates (PM10)	0.11	lb	0.11	kg
Particulates (PM2.5)	0.0098	lb	0.0098	kg
Particulates (unspecified)	0.031	lb	0.031	kg
Polyaromatic Hydrocarbons (total)	2.4E-05	lb	2.4E-05	kg
Sulfur Dioxide	1.54	lb	1.54	kg
Sulfur Oxides	0.0041	lb	0.0041	kg
Toluene	0.11	lb	0.11	kg
VOC	0.59	lb	0.59	kg
Xylene	0.066	lb	0.066	kg
Zinc	1.0E-06	lb	1.0E-06	kg
Solid Wastes				
Landfilled	34.1	lb	34.1	kg
Burned	7.63	lb	7.63	kg
Waste-to-Energy	0.0044	lb	0.0044	kg
Waterborne Wastes				
m-Xylene	8.5E-06	lb	8.5E-06	kg
1-Methylfluorene	1.7E-08	lb	1.7E-08	kg
2,4-Dimethylphenol	8.1E-06	lb	8.1E-06	kg
2-Hexanone	1.9E-06	lb	1.9E-06	kg
2-Methylnaphthalene	4.4E-06	lb	4.4E-06	kg
4-Methyl-2-Pentanone	6.4E-07	lb	6.4E-07	kg
Acetone	1.5E-06	lb	1.5E-06	kg
Acid (benzoic)	2.9E-04	lb	2.9E-04	kg
Acid (hexanoic)	6.1E-05	lb	6.1E-05	kg
Alkylated benzenes	5.5E-05	lb	5.5E-05	kg
Alkylated fluorenes	3.2E-06	lb	3.2E-06	kg
Alkylated naphthalenes	9.0E-07	lb	9.0E-07	kg
Alkylated phenanthrenes	3.7E-07	lb	3.7E-07	kg
Aluminum	0.027	lb	0.027	kg
Ammonia	0.0096	lb	0.0096	kg
Antimony	1.7E-05	lb	1.7E-05	kg
Arsenic	5.6E-05	lb	5.6E-05	kg
Barium	0.36	lb	0.36	kg
Benzene	3.2E-04	lb	3.2E-04	kg
Beryllium	3.5E-06	lb	3.5E-06	kg
BOD	0.046	lb	0.046	kg
Boron	9.1E-04	lb	9.1E-04	kg
Bromide	0.036	lb	0.036	kg
Cadmium	8.7E-06	lb	8.7E-06	kg
Calcium	0.60	lb	0.60	kg
Chlorides	7.44	lb	7.44	kg

Table E-1

DATA FOR THE PRODUCTION OF POLYPROPYLENE (PP) RESIN
(Cradle-to-Resin)
(page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Chromium (unspecified)	7.2E-04	lb	7.2E-04	kg
Cobalt	6.4E-06	lb	6.4E-06	kg
COD	0.17	lb	0.17	kg
Copper	7.8E-05	lb	7.8E-05	kg
Cyanide	1.1E-08	lb	1.1E-08	kg
Dibenzofuran	2.9E-08	lb	2.9E-08	kg
Dibenzothiophene	2.4E-08	lb	2.4E-08	kg
Dissolved Solids	7.57	lb	7.57	kg
Ethylbenzene	2.7E-05	lb	2.7E-05	kg
Fluorene	1.5E-06	lb	1.5E-06	kg
Iron	0.050	lb	0.050	kg
Lead	1.5E-04	lb	1.5E-04	kg
Lead 210	3.0E-14	lb	3.0E-14	kg
Lithium	0.11	lb	0.11	kg
Magnesium	0.12	lb	0.12	kg
Manganese	1.7E-04	lb	1.7E-04	kg
Mercury	3.2E-07	lb	3.2E-07	kg
Methyl Chloride	6.2E-09	lb	6.2E-09	kg
Methyl Ethyl Ketone	1.2E-08	lb	1.2E-08	kg
Molybdenum	6.7E-06	lb	6.7E-06	kg
Naphthalene	5.3E-06	lb	5.3E-06	kg
n-Decane	8.4E-06	lb	8.4E-06	kg
n-Docosane	1.6E-07	lb	1.6E-07	kg
n-Dodecane	1.6E-05	lb	1.6E-05	kg
n-Eicosane	4.4E-06	lb	4.4E-06	kg
n-Hexacosane	1.0E-07	lb	1.0E-07	kg
n-Hexadecane	1.7E-05	lb	1.7E-05	kg
Nickel	6.7E-05	lb	6.7E-05	kg
n-Octadecane	4.3E-06	lb	4.3E-06	kg
p -Xylene	3.1E-06	lb	3.1E-06	kg
o -Xylene	3.1E-06	lb	3.1E-06	kg
o-Cresol	8.3E-06	lb	8.3E-06	kg
Oil	0.0098	lb	0.0098	kg
p-Cresol	9.0E-06	lb	9.0E-06	kg
p-Cymene	1.5E-08	lb	1.5E-08	kg
Pentamethylbenzene	1.1E-08	lb	1.1E-08	kg
Phenanthrene	2.3E-07	lb	2.3E-07	kg
Phenol/ Phenolic Compounds	0.0012	lb	0.0012	kg
Tetradecane	6.8E-06	lb	6.8E-06	kg
Radium 226	1.0E-11	lb	1.0E-11	kg
Radium 228	5.4E-14	lb	5.4E-14	kg
Selenium	3.9E-06	lb	3.9E-06	kg
Silver	3.7E-04	lb	3.7E-04	kg
Sodium	1.73	lb	1.73	kg
Strontium	0.016	lb	0.016	kg
Styrene	1.0E-06	lb	1.0E-06	kg
Sulfates	0.012	lb	0.012	kg
Sulfides	7.9E-05	lb	7.9E-05	kg
Sulfur	7.2E-04	lb	7.2E-04	kg
Surfactants	1.5E-04	lb	1.5E-04	kg
Suspended Solids	2.99	lb	2.99	kg
Thallium	3.5E-06	lb	3.5E-06	kg
Tin	6.7E-05	lb	6.7E-05	kg
Titanium	2.6E-04	lb	2.6E-04	kg
TOC	0.0010	lb	0.0010	kg
Toluene	3.9E-04	lb	3.9E-04	kg
Total biphenyls	3.5E-06	lb	3.5E-06	kg
Total dibenzothiophenes	1.1E-08	lb	1.1E-08	kg
Vanadium	3.1E-05	lb	3.1E-05	kg
Xylene, unspecified	1.4E-04	lb	1.4E-04	kg
Yttrium	1.9E-06	lb	1.9E-06	kg
Zinc	6.2E-04	lb	6.2E-04	kg

References: Tables B-2 through B-5, E-2 and E-3.

Source: Franklin Associates, A Division of ERG models

Table E-2

DATA FOR THE PRODUCTION OF PROPYLENE

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs (1)							
Refined Petroleum Products	357	lb			357	kg	
Processed Natural Gas	643	lb			643	kg	
Water Consumption	161	gal			1,344	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	46.2	kwh		492	102	kwh	1.15
Electricity (cogeneration)	142	cu ft	(3)	159	8.85	cu meters	0.37
Natural Gas	1,759	cu ft		1,970	110	cu meters	4.59
Gasoline	0.0021	gal		0.29	0.017	liter	6.8E-04
Diesel	0.0018	gal		0.28	0.015	liter	6.6E-04
Internal Offgas use (2)							
From Oil	66.2	lb		1,884	66.2	kg	4.39
From Natural Gas	118	lb		3,350	118	kg	7.80
Recovered Energy	2.30	thousand Btu		2.30	5.35	MJ	0.0054
Total Process				7,853			18.3
Transportation Energy							
Propylene Products							
Pipeline-Petroleum Products	19.5	ton-miles			62.8	tonne-km	
Electricity	0.43	kwh		4.35	0.94	kwh	0.010
Environmental Emissions							
Atmospheric Emissions - Process							
Carbon Monoxide	0.0010	lb	(4)		0.0010	kg	
Chlorine	1.0E-04	lb	(4)		1.0E-04	kg	
HCFC-022	1.0E-06	lb	(4)		1.0E-06	kg	
Hydrogen Chloride	1.0E-06	lb	(4)		1.0E-06	kg	
Hydrogen	0.0052	lb			0.0052	kg	
Hydrocarbons (NM)	0.11	lb			0.11	kg	
Methane	0.0010	lb	(4)		0.0010	kg	
Other Organics	0.0010	lb	(4)		0.0010	kg	
Particulates (unspecified)	0.0082	lb			0.0082	kg	
Particulates (PM10)	0.10	lb	(4)		0.10	kg	
Sulfur Oxides	0.0041	lb			0.0041	kg	
VOC	0.010	lb	(4)		0.010	kg	
Atmospheric Emissions - Fuel-Related (5)							
Carbon Dioxide (fossil)	666	lb			666	kg	
Carbon Monoxide	0.30	lb			0.30	kg	
Nitrogen Oxides	0.47	lb			0.47	kg	
PM 2.5	0.009	lb			0.009	kg	
Sulfur Oxides	0.071	lb			0.071	kg	
Solid Wastes							
Landfilled	0.36	lb			0.36	kg	
Burned	5.60	lb			5.60	kg	
Waste-to-Energy	0.0044	lb			0.0044	kg	
Waterborne Wastes							
Acetone	1.0E-08	lb	(4)		1.0E-08	kg	
Benzene	1.0E-05	lb	(4)		1.0E-05	kg	
BOD	6.4E-04	lb			6.4E-04	kg	
COD	0.010	lb	(4)		0.010	kg	
Ethylbenzene	1.0E-05	lb	(4)		1.0E-05	kg	
Naphthalene	1.0E-08	lb	(4)		1.0E-08	kg	
Phenol	0.0010	lb	(4)		0.0010	kg	
Styrene	1.0E-06	lb	(4)		1.0E-06	kg	
Suspended Solids	0.0048	lb			0.0048	kg	
Toluene	1.0E-04	lb	(4)		1.0E-04	kg	
Total Organic Carbon	0.0010	lb	(4)		0.0010	kg	
Xylene	1.0E-06	lb	(4)		1.0E-06	kg	

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(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.

(3) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(4) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(5) These fuel-related emissions were provided by the plants. These take into account the combustion of the offgas as well as the natural gas.

References: E-3 and E-4

Source: Franklin Associates, A Division of ERG

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

where
IO = Input/Output Matrix to produce all products/coproducts
M_{EO} = Mass of Exported Offgas
M_{Total} = Mass of all Products and Coproducts (including fuels)

No energy credit is applied for the exported fuels, since both the inputs and outputs for the exported fuels have been removed from the data set. Table E-2 shows the averaged energy and emissions data for the production of propylene.

As of 2003, there were 8 olefin-producing companies and at least 16 olefin plants producing polymer-grade propylene in the U.S. (Reference E-2). While data was collected from a relatively small sample of plants, the olefins producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American olefins production. All data collected were individually reviewed by the data providers.

To assess the quality of the data collected for olefins, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for olefins include direct measurements, information provided by purchasing and utility records, and estimates. The standard production technology for olefins is the steam cracking of hydrocarbons (including natural gas liquids and petroleum liquids). The data in this module represent steam cracking of natural gas and petroleum. All data submitted for olefins represent the year 2003 and U.S. and Canada production.

Polypropylene Resin Production

Polypropylene is manufactured by the polymerization of propylene using Ziegler-Natta catalysts. Commercial processes generally use titanium trichloride in combination with aluminum diethylmonochloride. Production processes vary and include slurry, gas-phase, and solution monomer polymerization. The latter two processes employ the use of improved high-yield catalysts. The five polypropylene datasets represent the gas-phase and solution monomer polymerization processes. These processes are discussed below.

The gas-phase method of production mixes the high-yield type catalyst and propylene vapor in a fluidized bed or agitated powder bed reactor. Temperature control is accomplished by the evaporation of liquid propylene entering the reactor. Reactor temperatures of 80° to 90° Celsius and pressures of 30 to 35 atmospheres are typical. Unreacted propylene gas is recovered, compressed, purified, and returned to the propylene feed stream. The polymer is then dried and pelletized. Catalyst residues are low and catalyst removal is not part of this process. No solvent is used in the process; therefore, no solvent recovery is necessary.

The solution monomer process of manufacturing polypropylene often employs tubular reactors with a large specific-exchange surface and a high heat-exchange coefficient. The use of high-yield catalyst eliminates the need for catalyst residue and atactic removal. Unreacted propylene is recovered, and the isotactic polypropylene is dried and pelletized. As in the gas-phase process, no solvent is used.

A weighted average using production amounts was calculated from the PP production data from four plants collected from three leading producers in North America. Table E-3 displays the energy and emissions data for the production of polypropylene resin. Scrap and some alkane/alkene streams are produced as coproducts during this process. A mass basis was used to partition the credit for the coproducts.

As of 2003 there were 11 PP producers and 20 PP plants in the U.S. (Reference E-5). While data was collected from a small sample of plants, the PP producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American PP production. The average dataset was reviewed and accepted by all PP data providers.

To assess the quality of the data collected for PP, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for PP include direct measurements, information provided by purchasing and utility records, and estimates. The technology represented by the PP data represents a combination of the liquid monomer and gas phase processes. All data submitted for PP represent the years 2003 and 2004 and production in U.S.

Table E-3

DATA FOR THE PRODUCTION OF POLYPROPYLENE (PP) RESIN

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Olefins	996	lb			996	kg	
Propane	5.0	lb			5.0	kg	
Water Consumption	139	gal			1,160	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	74.0	kwh		762	163	kwh	1.77
Electricity (cogeneration)	453	cu ft	(1)	507	28.3	cu meters	1.18
Natural gas	310	cu ft		347	19.4	cu meters	0.81
Residual oil	0.52	gal		89.2	4.34	liter	0.21
Total Process				1,705			3.97
Environmental Emissions							
Atmospheric Emissions							
Carbon Monoxide	0.12	lb			0.12	kg	
Carbon Dioxide	19.3	lb			19.3	kg	
Lead	1.0E-12	lb	(2)		1.0E-12	kg	
Methane	0.068	lb			0.068	kg	
Nitrogen Oxides	0.014	lb			0.014	kg	
Nitrous Oxides	0.0045	lb			0.0045	kg	
NM Hydrocarbons	0.15	lb			0.15	kg	
Other Organics	0.010	lb	(2)		0.010	kg	
Particulates (unknown)	0.023	lb			0.023	kg	
PM2.5	1.0E-05	lb	(2)		1.0E-05	kg	
PM10	0.0010	lb	(2)		0.0010	kg	
Sulfur Oxides	1.0E-04	lb	(2)		1.0E-04	kg	
Zinc	1.0E-06	lb	(2)		1.0E-06	kg	
Solid Wastes							
Landfilled	0.11	lb			0.11	kg	
Burned	2.06	lb			2.06	kg	
Waterborne Wastes							
BOD	0.0010	lb	(2)		0.0010	kg	
COD	0.010	lb	(2)		0.010	kg	
Dissolved solids	0.010	lb	(2)		0.010	kg	
Suspended Solids	0.020	lb			0.020	kg	
Zinc	1.0E-05	lb	(2)		1.0E-05	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

References: E-4

Source: Franklin Associates, A Division of ERG

REFERENCES

E-1. APC Plastics Industry Producers' Statistics Group, as compiled by VERIS Consulting, LLC. 2004.

E-2. Chemical Profile: Propylene. **Chemical Market Reporter.** October 6, 2003. Page 23.

E-3. Information and data collected from APC member and non-member companies producing olefins. 2004-2005.

E-4. Information and data collected from APC member and non-member companies producing PP. 2004-2005.

E-5. Chemical profile information taken from the website: http://www.the-innovation-group.com/welcome.htm.

APPENDIX F

POLYETHYLENE TEREPHTHALATE (PET)

INTRODUCTION

This appendix discusses the manufacture of polyethylene terephthalate (PET) resin. The leading use of PET resin is bottle production. Over 7 billion pounds of PET was produced in the U.S., Mexico, and Canada in 2003 (Reference F-1). The material flow for PET resin is shown in Figure F-1. The total unit process energy and emissions data (cradle-to-PET) for PET are displayed in Table F-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following processes are included in this appendix:

- Methanol Production
- Carbon Monoxide Production
- Acetic Acid Production
- Oxygen Production
- Ethylene Oxide Production
- Ethylene Glycol Production
- Mixed Xylenes
- Paraxylene Extraction
- Crude Terephthalic Acid (TPA) Production
- Purified TPA (PTA) Production
- Dimethyl Terephthalate (DMT) Production
- PET Melt Phase Polymerization
- PET Solid Phase Polymerization

Crude oil production, distillation, desalting, and hydrotreating, natural gas production, natural gas processing, and ethylene production are discussed in Appendix B.

Methanol Production

Methanol is produced from light hydrocarbons using steam reforming and low-pressure synthesis. The feed gas is compressed, preheated, and desulfurized. Then, it is mixed with steam, preheated further, and fed to the catalytic reformer. The synthesis gas from the reformer, containing primarily hydrogen, carbon monoxide, and carbon dioxide, is cooled to remove condensate to the proper temperature for entry into the compressor section.

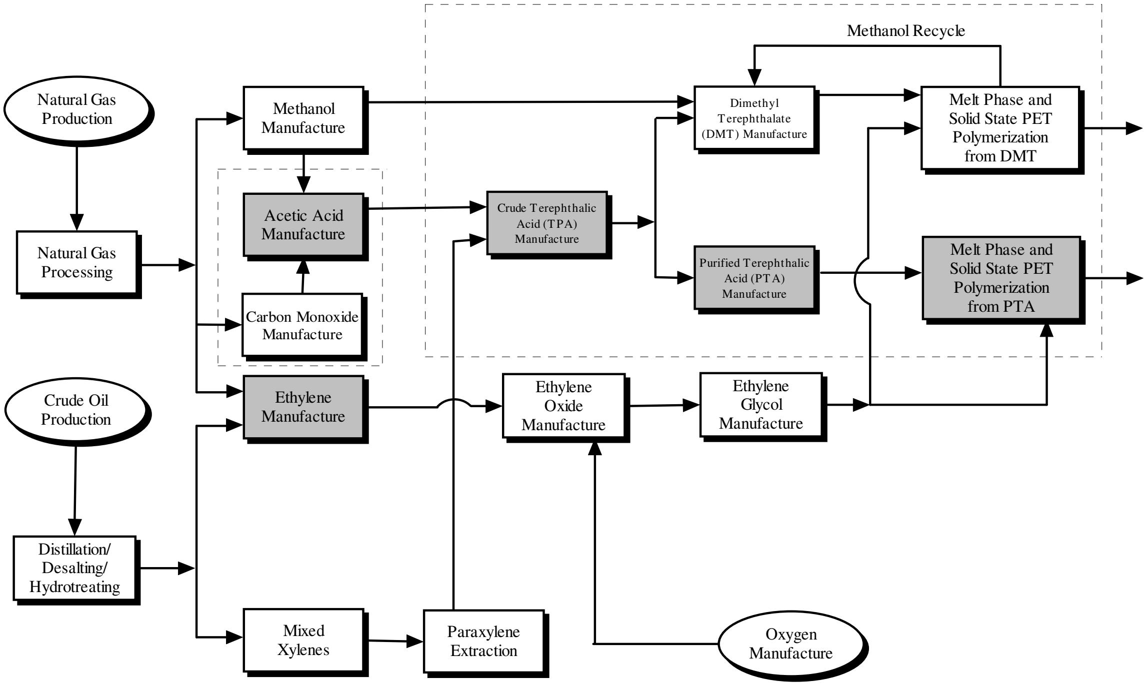

Figure F-1. Flow diagram for the manufacture of virgin polyethylene terephthalate(PET) resin. Shaded boxes represent partial or complete data provided by manufacturers specifically for this analysis. Boxes within the dotted rectangle are included in an aggregated dataset.

From the compressor, the pressure of the synthesis gas is raised, and the feed goes to a multi-bed inter-cooled methanol converter system. Converter effluent is sent to a cooler, and the crude methanol is removed from the gas mixture. The crude methanol is then brought to atmospheric pressure and distilled to eliminate dissolved gases and obtain the desired grade.

Table F-2 lists the energy requirements and environmental emissions for the manufacture of 1,000 pounds of methanol. Steam production is included in energy use for methanol production. The energy and carbon dioxide data for methanol are from a source outside of the United States. No energy and carbon dioxide data for the production of methanol are available for the United States. Waterborne emissions data are provided by an older U.S. source and may be overstated. The transportation energy was collected from an acetic acid producer and calculated using estimates.

Table F-1

DATA FOR THE PRODUCTION
OF POLYETHYLENE TEREPHTHALATE (PET) RESIN
(Cradle-to-Resin)
(page 1 of 4)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	568	lb		568	kg	
Natural Gas	215	lb		215	kg	
Oxygen	223	lb		223	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			4,595			10.7
Petroleum			10,666			24.8
Total Resource			15,262			35.5
Process Energy						
Electricity (grid)	400	kwh	4,255	882	kwh	9.91
Electricity (cogeneration)	194	cu ft (2)	218	12.1	cu meters	0.51
Natural gas	5,640	cu ft	6,317	352	cu meters	14.7
LPG	0.68	gal	73.9	5.70	liter	0.17
Bit./Sbit. Coal	35.9	lb	404	35.9	kg	0.94
Distillate oil	1.65	gal	263	13.8	liter	0.61
Residual oil	9.60	gal	1,648	80.1	liter	3.84
Gasoline	0.070	gal	10.0	0.59	liter	0.023
Diesel	0.0019	gal	0.30	0.016	liter	7.0E-04
Internal Offgas use (1)						
From Oil	5.22	lb	160	5.22	kg	0.37
From Natural Gas	23.8	lb	729	23.8	kg	1.70
Recovered Energy	63.5	thousand Btu	63.5	148	MJ	0.15
Total Process			14,013			32.6
Transportation Energy						
Combination truck	8.85	ton-miles		28.5	tonne-km	
Diesel	0.093	gal	14.8	0.78	liter	0.034
Rail	507	ton-miles		1,633	tonne-km	
Diesel	1.26	gal	200	10.5	liter	0.46
Barge	43.1	ton-miles		139	tonne-km	
Diesel	0.034	gal	5.48	0.29	liter	0.013
Residual oil	0.11	gal	19.7	0.96	liter	0.046
Ocean freighter	844	ton-miles		2,717	tonne-km	
Diesel	0.16	gal	25.5	1.34	liter	0.059
Residual	1.44	gal	248	12.0	liter	0.58
Pipeline-natural gas	119	ton-miles		382	tonne-km	
Natural gas	81.9	cu ft	91.8	5.11	cu meter	0.21
Pipeline-petroleum products	185	ton-miles		595	tonne-km	
Electricity	4.03	kwh	41.3	8.89	kwh	0.096
Total Transportation			646			1.50

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table F-1

DATA FOR THE PRODUCTION
OF POLYETHYLENE TEREPHTHALATE (PET) RESIN
(Cradle-to-Resin)
(page 2 of 4)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Acetic Acid	0.051	lb	0.051	kg
Aldehydes (unspecified)	0.17	lb	0.17	kg
Ammonia	0.0020	lb	0.0020	kg
Antimony	1.1E-06	lb	1.1E-06	kg
Arsenic	1.4E-07	lb	1.4E-07	kg
Benzene	0.023	lb	0.023	kg
Bromine	0.079	lb	0.079	kg
Carbon Dioxide - Fossil	294	lb	294	kg
Carbon Monoxide	6.06	lb	6.06	kg
Carbon Tetrachloride	7.7E-07	lb	7.7E-07	kg
CFC 13 (Methane, trichlorofluoro-)	1.2E-05	lb	1.2E-05	kg
Chlorine	2.0E-05	lb	2.0E-05	kg
Chromium	3.8E-07	lb	3.8E-07	kg
Ethylbenzene	0.0027	lb	0.0027	kg
Ethylene Dibromide	2.4E-06	lb	2.4E-06	kg
Ethylene Oxide	0.024	lb	0.024	kg
HCFC-22	2.0E-07	lb	2.0E-07	kg
Hydrogen	7.9E-04	lb	7.9E-04	kg
Hydrogen Chloride	2.0E-07	lb	2.0E-07	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.38	lb	0.38	kg
Methane	5.25	lb	5.25	kg
Methanol	0.0015	lb	0.0015	kg
Methyl Acetate	0.040	lb	0.040	kg
Nickel	3.2E-06	lb	3.2E-06	kg
Nitrogen Oxides	0.29	lb	0.29	kg
Non-Methane Hydrocarbons	5.57	lb	5.57	kg
Other Organics	1.11	lb	1.11	kg
Particulates (PM10)	0.038	lb	0.038	kg
Particulates (PM2.5)	0.013	lb	0.013	kg
Particulates (unspecified)	0.15	lb	0.15	kg
Polyaromatic Hydrocarbons (total)	3.1E-05	lb	3.1E-05	kg
Sulfur Dioxide	0.59	lb	0.59	kg
Sulfur Oxides	0.0015	lb	0.0015	kg
TOC	0.069	lb	0.069	kg
Toluene	0.035	lb	0.035	kg
VOC	0.18	lb	0.18	kg
Xylene	0.062	lb	0.062	kg
Solid Wastes				
Landfilled	32.9	lb	32.9	kg
Burned	1.03	lb	1.03	kg
Waste-to-Energy	0.59	lb	0.59	kg
Waterborne Wastes				
m-Xylene	5.4E-06	lb	5.4E-06	kg
1-Methylfluorene	7.7E-09	lb	7.7E-09	kg
2,4-Dimethylphenol	5.3E-06	lb	5.3E-06	kg
2-Hexanone	1.2E-06	lb	1.2E-06	kg
2-Methylnaphthalene	2.8E-06	lb	2.8E-06	kg
4-Methyl-2-Pentanone	2.9E-07	lb	2.9E-07	kg
Acetaldehyde	0.025	lb	0.025	kg
Acetone	6.8E-07	lb	6.8E-07	kg
Acid (benzoic)	1.9E-04	lb	1.9E-04	kg
Acid (hexanoic)	3.9E-05	lb	3.9E-05	kg
Acid (unspecified)	0.036	lb	0.036	kg
Alkylated benzenes	3.6E-05	lb	3.6E-05	kg
Alkylated fluorenes	2.1E-06	lb	2.1E-06	kg
Alkylated naphthalenes	5.9E-07	lb	5.9E-07	kg
Alkylated phenanthrenes	2.4E-07	lb	2.4E-07	kg
Aluminum	0.018	lb	0.018	kg
Ammonia	0.12	lb	0.12	kg
Ammonium	0.0013	lb	0.0013	kg
Antimony	1.2E-05	lb	1.2E-05	kg
Arsenic	3.8E-05	lb	3.8E-05	kg
Barium	0.24	lb	0.24	kg
Benzene	2.1E-04	lb	2.1E-04	kg
Beryllium	2.4E-06	lb	2.4E-06	kg
BOD	0.91	lb	0.91	kg
Boron	5.9E-04	lb	5.9E-04	kg
Bromide	0.025	lb	0.025	kg
Cadmium	5.8E-06	lb	5.8E-06	kg

Table F-1

DATA FOR THE PRODUCTION
OF POLYETHYLENE TEREPHTHALATE (PET) RESIN
(Cradle-to-Resin)
(page 3 of 4)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Calcium	0.41	lb	0.41	kg
Chlorides	4.99	lb	4.99	kg
Chromium (unspecified)	0.0068	lb	0.0068	kg
Cobalt	4.2E-06	lb	4.2E-06	kg
COD	1.64	lb	1.64	kg
Copper	5.1E-05	lb	5.1E-05	kg
Cyanide	4.9E-09	lb	4.9E-09	kg
Dibenzofuran	1.3E-08	lb	1.3E-08	kg
Dibenzothiophene	1.0E-08	lb	1.0E-08	kg
Dissolved Solids	5.23	lb	5.23	kg
Ethylbenzene	1.4E-05	lb	1.4E-05	kg
Fluorides	5.1E-05	lb	5.1E-05	kg
Fluorene	9.7E-07	lb	9.7E-07	kg
Iron	0.033	lb	0.033	kg
Lead	9.8E-05	lb	9.8E-05	kg
Lead 210	2.0E-14	lb	2.0E-14	kg
Lithium	0.036	lb	0.036	kg
Magnesium	0.081	lb	0.081	kg
Manganese	1.2E-04	lb	1.2E-04	kg
Mercury	2.3E-07	lb	2.3E-07	kg
Metal Ion (unspecified)	4.5E-06	lb	4.5E-06	kg
Methyl Chloride	2.7E-09	lb	2.7E-09	kg
Methyl Ethyl Ketone	5.5E-09	lb	5.5E-09	kg
Molybdenum	4.3E-06	lb	4.3E-06	kg
Naphthalene	3.4E-06	lb	3.4E-06	kg
n-Decane	5.4E-06	lb	5.4E-06	kg
n-Docosane	7.3E-08	lb	7.3E-08	kg
n-Dodecane	1.0E-05	lb	1.0E-05	kg
n-Eicosane	2.8E-06	lb	2.8E-06	kg
n-Hexacosane	4.5E-08	lb	4.5E-08	kg
n-Hexadecane	1.1E-05	lb	1.1E-05	kg
Nickel	4.5E-05	lb	4.5E-05	kg
n-Octadecane	2.8E-06	lb	2.8E-06	kg
p -Xylene	2.0E-06	lb	2.0E-06	kg
o -Xylene	2.0E-06	lb	2.0E-06	kg
o-Cresol	5.4E-06	lb	5.4E-06	kg
Oil	0.0095	lb	0.0095	kg
p-Cresol	5.8E-06	lb	5.8E-06	kg
p-Cymene	6.8E-09	lb	6.8E-09	kg
Pentamethylbenzene	5.1E-09	lb	5.1E-09	kg
Phenanthrene	1.5E-07	lb	1.5E-07	kg
Phenol/ Phenolic Compounds	3.9E-04	lb	3.9E-04	kg
Phosphates	5.1E-04	lb	5.1E-04	kg

Table F-1

DATA FOR THE PRODUCTION
OF POLYETHYLENE TEREPHTHALATE (PET) RESIN
(Cradle-to-Resin)
(page 4 of 4)

	English units (Basis: 1,000 lb)	SI units (Basis: 1,000 kg)
Tetradecane	4.3E-06 lb	4.3E-06 kg
Radium 226	6.8E-12 lb	6.8E-12 kg
Radium 228	3.5E-14 lb	3.5E-14 kg
Selenium	3.0E-06 lb	3.0E-06 kg
Silver	2.5E-04 lb	2.5E-04 kg
Sodium	1.19 lb	1.19 kg
Strontium	0.010 lb	0.010 kg
Styrene	2.0E-07 lb	2.0E-07 kg
Sulfates	0.0085 lb	0.0085 kg
Sulfides	1.0E-04 lb	1.0E-04 kg
Sulfur	4.6E-04 lb	4.6E-04 kg
Surfactants	9.9E-05 lb	9.9E-05 kg
Suspended Solids	2.02 lb	2.02 kg
Thallium	2.3E-06 lb	2.3E-06 kg
Tin	4.3E-05 lb	4.3E-05 kg
Titanium	1.7E-04 lb	1.7E-04 kg
TOC	0.044 lb	0.044 kg
Toluene	2.2E-04 lb	2.2E-04 kg
Total biphenyls	2.3E-06 lb	2.3E-06 kg
Total dibenzothiophenes	7.2E-09 lb	7.2E-09 kg
Vanadium	3.5E-05 lb	3.5E-05 kg
Xylene, unspecified	9.4E-05 lb	9.4E-05 kg
Yttrium	1.3E-06 lb	1.3E-06 kg
Zinc	0.0084 lb	0.0084 kg

References: Tables B-2 through B-6 and F-2 through F-8.

Source: Franklin Associates, A Division of ERG models

Carbon Monoxide Production

The raw materials necessary for the production of carbon monoxide are the gases resulting from steam reformation, as in the production of synthesis gas for ammonia manufacture, or from partial combustion of hydrocarbons. The feed gas must be stripped of carbon dioxide by scrubbing with ethanolamine solution and then passed through a molecular sieve to remove traces of carbon dioxide and water. Carbon monoxide and unconverted methane are condensed from the gas mixture and separated by lowering the pressure to remove entrained gases. The methane is recycled and the carbon monoxide comes out as a product after evaporation, warming, and compression.

The energy requirements and environmental emissions for the production of carbon monoxide using steam reformation are included in the production of acetic acid (Table F-3). The energy and emissions data for carbon monoxide are from secondary sources and estimates. The transportation energy was collected from an acetic acid producer and calculated using estimates.

Table F-2

DATA FOR THE PRODUCTION OF METHANOL

	English units (Basis: 1,000 lb)		Total Energy Thousand Btu	SI units (Basis: 1,000 kg)		Total Energy GigaJoules
Material Inputs						
Oxygen, from air	380	lb		380	kg	
Natural Gas	620	lb		620	kg	
Water Consumption	142	gal		1189	liter	
Energy Usage						
Process Energy						
Electricity (grid)	3.65	kwh	38	8.04	kwh	0.087
Natural gas	2,081	cu ft	2,330	130	cu meters	5.43
Total Process			2,368			5.51
Transportation Energy						
Barge	25.0	ton-miles		80.5	tonne-km	
Diesel	0.020	gal	3.2	0.17	liter	0.0074
Residual oil	0.067	gal	11.4	0.55	liter	0.027
Pipeline-natural gas	0.50	ton-miles		1.61	tonne-km	
Natural gas	0.35	cu ft	0.4	0.022	cu meter	9.0E-04
Total Transportation			15.0			0.035
Environmental Emissions						
Atmospheric Emissions						
Hydrocarbons	5.0	lb		5.0	kg	
Carbon Dioxide	530	lb		530	kg	
Solid Wastes						
Landfilled	0.50	lb		0.50	kg	
Waterborne Wastes						
BOD	0.058	lb		0.058	kg	
Suspended solids	0.088	lb		0.088	kg	

References: F-2 through F-5, F-7 and F-22.

Source: Franklin Associates, A Division of ERG

Acetic Acid Production

Several methods are used for producing acetic acid. Some methods used in the United States include liquid phase oxidation of butane or LPG and the oxidation of acetaldehyde. Most commercial production of virgin synthetic acetic acid is made by reacting carbon monoxide with methanol. Recovered acetic acid represents an additional major supply (Reference F-2).

Table F-3 shows the energy and emissions data for producing acetic acid. Mixed acid and offgas are produced as coproducts during this process. A mass basis was used to partition the credit for the acid. When the offgas is exported from the process, it carries with it the allocated share of the inputs and outputs for its production. The ratio of the mass of the exported fuel 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).

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

where
IO = Input/Output Matrix to produce all products/coproducts
M_{EO} = Mass of Exported Offgas
M_{Total} = Mass of all Products and Coproducts (including fuels)

No energy credit is applied for the exported offgas, since both the inputs and outputs for the exported fuel have been removed from the data set.

The data in Table F-3 represents the production of acetic acid by the carbonylation of methanol. As only 2 confidential datasets were available, the carbon monoxide dataset is included within the acetic acid data. One of these datasets was collected for this project and represents 2003 data in the U.S., while the other U.S. dataset comes from 1994. As no production amounts were available for either datasets, an arithmetic average was used to weight the data. The 2003 data were collected from direct measurements and engineering estimates.

Oxygen Production

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

The energy data for producing oxygen is displayed in Table F-4. This energy data is primary data collected from 3 producers representing air separation for the years 1990 through 1993.

Table F-3

DATA FOR THE PRODUCTION OF ACETIC ACID
(Includes acetic acid and carbon monoxide data)

	English units (Basis: 1,000 lb)		Total Energy Thousand Btu	SI units (Basis: 1,000 kg)		Total Energy GigaJoules
Material Inputs						
Methanol	539	lb		539	kg	
Natural Gas products	353	lb		353	kg	
Water, from nature	332	lb		332	kg	
Energy Usage						
Process Energy						
Electricity (grid)	27.4	kwh	282	60.4	kwh	0.66
Electricity (cogeneration)	6.16	cu ft (1)	6.90	0.38	cu meters	0.016
Natural gas	4,348	cu ft	4,870	271	cu meters	11.3
Total Process			5,159			12.0
Transportation Energy						
Rail	475	ton-miles		1,529	tonne-km	
Diesel	1.18	gal	187	9.83	liter	0.44
Pipeline-natural gas	0.26	ton-miles		0.83	tonne-km	
Natural gas	0.18	cu ft	0.20	0.011	cu meter	0.0005
Total Transportation			187			0.44
Environmental Emissions						
Atmospheric Emissions						
Carbon Monoxide	3.61	lb		3.61	kg	
Sulfur Oxides	0.015	lb		0.015	kg	
TOC	1.86	lb		1.86	kg	
Methanol	0.040	lb		0.040	kg	
Solid Wastes						
Landfilled	0.46	lb		0.46	kg	
Waterborne Wastes						
Acid (unspecified)	0.96	lb		0.96	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

References: F-2, F-4, and F-6 through F-10.

Source: Franklin Associates, A Division of ERG

Table F-4

DATA FOR THE PRODUCTION OF OXYGEN

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	62.6	kwh	644	138	kwh	1.50
Total Process			644			1.50
Transportation Energy						
Pipeline-natural gas	0.50	ton-miles		1.61	tonne-km	
Natural gas	0.35	cu ft	0.39	0.022	cu meter	9.0E-04
Total Transportation			0.39			9.0E-04

References: F-4 and F-11

Source: Franklin Associates, A Division of ERG

Ethylene Oxide Production

The primary production method for ethylene oxide is the direct oxidation of ethylene using air or oxygen. The predominant feed for commercial oxidation processes is oxygen rather than air. The reaction is catalyzed by silver and is exothermic. Oil or boiling water is used to absorb the heat in a multitubular reactor and produce steam that is used in other parts of the process.

A disadvantage to the oxidation process is the conversion of ethylene to carbon dioxide and water, which is released to the environment. Excess ethylene is added to prevent additional oxidation of the ethylene oxide that would increase the production of carbon dioxide. This creates typical conversion rates for ethylene to ethylene oxide of only 10 to 20 percent per pass. Approximately 20 to 25 percent of the ethylene is broken down to carbon dioxide and water.

The energy requirements and environmental emissions for the production of ethylene oxide are shown in Table F-5. These data are a straight average of 6 ethylene oxide producers in the U.S. and Europe from 1990 through 1992. This average data was sent to a Plastics Division of the American Chemistry Council (ACC) member company that produces ethylene oxide for review. The company agreed that the energy and emissions are acceptable for 2005; however, new raw material estimates were provided by the Plastics Division of the American Chemistry Council (ACC) member company.

Ethylene Glycol Production

Ethylene glycol is produced by the hydration of ethylene oxide. The production process is generally close to the process unit for ethylene oxide. Ethylene oxide is very hazardous to handle and transport. In this case, crude oxide solution is used as feed to the glycol unit. Using crude solution avoids a refining step but still provides an adequate feed.

An excess amount of water is added to the reactor feed to reduce the amount of diethylene glycol and triethylene glycol. These glycols are produced from the reaction of monoethylene glycol with ethylene oxide. The hydration reaction can be uncatalyzed or catalyzed with an acid. An uncatalyzed reaction is much slower, but acid removal from the glycol is required if a catalyst is used.

Almost all the ethylene oxide is reacted. This glycol/water mixture is sent through an evaporator to concentrate the solution and recover the water. The water is recycled back to be used to prepare the ethylene oxide feed. High purity ethylene glycol is obtained from the concentrated glycol solution by vacuum distillation.

The energy and emissions data for ethylene glycol production is from a confidential source and is not shown to protect its confidentiality (Reference F-14).

Table F-5

DATA FOR THE PRODUCTION OF ETHYLENE OXIDE

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Ethylene	788	lb		788	kg	
Oxygen	880	lb		880	kg	
Water Consumption	200	gal		1669	liter	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	101	kwh	1,041	223	kwh	2.42
Natural gas	1,618	cu ft	1,812	101	cu meters	4.22
Total Process			2,854			6.64
Transportation Energy Used in PET						
Pipeline-petroleum products	1.00	ton-miles		3.22	tonne-km	
Electricity	0.022	kwh	0.22	0.048	kwh	5.2E-04
Total Transportation			0.22			5.2E-04
Used in polyether polyol for flexible foam PUR						
Rail	12.4	ton-miles		39.9	tonne-km	
Diesel	0.031	gal	4.88	0.26	liter	0.011
Pipeline-petroleum products	0.31	ton-miles		1.00	tonne-km	
Electricity	0.0068	kwh	0.069	0.015	kwh	1.6E-04
Total Transportation			4.95			0.012
Environmental Emissions						
Atmospheric Emissions						
Aldehydes	0.28	lb		0.28	kg	
Carbon Monoxide	3.0E-04	lb		3.0E-04	kg	
Carbon Dioxide	591	lb		591	kg	
Ethylene Oxides	0.10	lb		0.095	kg	
Hydrocarbons	18.1	lb		18.1	kg	
Methane	3.05	lb		3.05	kg	
Nitrogen Oxides	0.0014	lb		0.0014	kg	
Other Organics	0.68	lb		0.68	kg	
Sulfur Oxides	3.0E-04	lb		3.0E-04	kg	
Solid Wastes	16.8	lb		16.8	kg	
Waterborne Wastes						
Acetaldehyde	0.10	lb		0.10	kg	
Ammonia	5.0E-05	lb		5.0E-05	kg	
BOD	2.23	lb		2.23	kg	
Chromium	0.025	lb		0.025	kg	
COD	2.82	lb		2.82	kg	
Fluorides	0.0002	lb		2.0E-04	kg	
Zinc	0.010	lb		0.010	kg	

References: F-2, F-4, F-12, and F-13.

Source: Franklin Associates, A Division of ERG

Mixed Xylenes

The reforming processes are used to convert paraffinic hydrocarbon streams into aromatic compounds such as benzene, toluene, and xylene. Catalytic reforming has virtually replaced thermal reforming operations. Catalytic reforming has many advantages over thermal reforming including the following:

1. Greater production of aromatics
2. More olefin isomerization
3. More selective reforming and fewer end products
4. Operated at a low pressure, hence comparatively lower cost.

Catalysts such as platinum, alumina, or silica-alumina and chromium on alumina are used.

Table F-6 displays the energy and emissions data for the production of mixed xylenes. Total energy data for mixed xylenes were provided for this analysis by a confidential source. The mix of fuels shown in Table F-6 was calculated using statistics from a U.S. Department of Energy report (Reference F-16). No environmental emissions data were available.

Table F-6

DATA FOR THE PRODUCTION OF MIXED XYLENES FROM NAPHTHA

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Naphtha	1,000	lb		1,000	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	16.1	kwh	166	35.5	kwh	0.39
Natural gas	667	cu ft	747	41.6	cu meters	1.74
LPG	0.25	gal	27.0	2.09	liter	0.063
Bit./Sbit. Coal	7.02	lb	78.8	7.02	kg	0.18
Total Process			1,019			2.37

References: F-4, F-15, and F-16.

Source: Franklin Associates, A Division of ERG

Paraxylene Extraction

Reformate feedstock rich in xylenes is fractionated to obtain a stream rich in the para-isomer. Further purification is accomplished by heat exchange and refrigeration. The solid paraxylene crystals are separated from the feedstock by centrifugation.

Table F-7 displays the energy requirements for the production of paraxylene. Total energy data for paraxylene were provided for this analysis by a confidential source. The mix of fuels shown in Table F-7 was calculated using statistics from a U.S. Department of Energy report (Reference F-16). No environmental emissions data were available.

Table F-7

DATA FOR THE EXTRACTION OF PARAXYLENE

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Mixed Xylenes	1,000	lb		1,000	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	59.0	kwh	607	130	kwh	1.41
Natural gas	2,445	cu ft	2,738	153	cu meters	6.37
LPG	0.91	gal	98.4	7.59	liter	0.23
Bit./Sbit. Coal	25.7	lb	289	25.7	kg	0.67
Total Process			3,733			8.69
Transportation Energy						
Rail	650	ton-miles		2,092	tonne-km	
Diesel	1.61	gal	256	13.5	liter	0.60
Total Transportation			256			0.60

References:F-2, F-4, F-16, and F-17.

Source: Franklin Associates, A Division of ERG

Crude Terephthalic Acid (TPA) Production

Crude terephthalic acid is manufactured primarily by the oxidation of paraxylene in the liquid phase. Liquid paraxylene, acetic acid, and a catalyst, such as manganese or cobalt bromides, are combined as the liquid feed to the oxidizers. The temperature of this exothermic reaction is maintained at about 200° C. The pressure may range from 300 to 400 psi.

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

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

Purified Terephthalic Acid (PTA) Production

There are two primary methods of crude TPA purification. The first, described here, is by direct production of fiber-grade TPA or purified terephthalic acid (PTA).

In the production of fiber-grade TPA from crude TPA, the crude acid is dissolved under pressure in water at 225 to 275° C. The solution is hydrogenated in the presence of a catalyst to convert some troublesome intermediates of reaction. The solution is then cooled, causing PTA to crystallize out.

Dimethyl Terephthalate (DMT) Production

The other primary method of crude TPA purification is by conversion of crude TPA to dimethyl terephthalate (DMT). DMT now makes up no more than 15 percent of the precursor s used for PET production within North America.

The common method for the production of DMT consists of four major steps: oxidation, esterification, distillation, and crystallization. A mixture of p-xylene and crude PTA is oxidized with air in the presence of a heavy metal catalyst. The acid mixture resulting from the oxidation is esterified with methanol to produce a mixture of esters. The crude ester mixture is distilled to remove all the heavy boilers and residue produced; the lighter esters are recycled to the oxidation section. The raw DMT is then sent to the crystallization section for removal of DMT isomers and aromatic aldehydes. Some byproducts are recovered, and usable materials are recycled (Reference F-21).

PET Melt Phase Polymerization

PET resin is manufactured by the esterification of PTA with ethylene glycol and loss of water, or by the trans-esterification of DMT with ethylene glycol and loss of methanol. Both reactions occur at 100 to 150° C in the presence of a catalyst. Bis (2-hydroxyethyl) terephthalate is produced as an intermediate. This intermediate then undergoes polycondensation under vacuum at 10 to 20° C above the melting point of PET (246° C). Ethylene glycol is distilled over, and PET resin with an I.V. (intrinsic viscosity) of 0.60 to 0.65 is produced. The resulting resin is cooled and pelletized.

PET Solid State Polymerization

The final step in PET resin manufacture is a solid state polymerization process. This step raises the temperature of the solid pellets to just below the melting point in the presence of a driving force to further the polymerization. Solid stating increases the final I.V. from 0.72 to 1.04. It also produces a polymer with low acetaldehyde content.

Table F-8 shows the combined energy usage and environmental emissions for the melt phase and the solid state polymerization steps for production of PET from both PTA and DMT. Scrap and heat are produced as coproducts during this process. A mass basis was used to partition the credit for scrap, while the energy amount for the steam was reported separately as recovered energy.

The data in this table includes an aggregation of TPA, PTA, DMT, and PET production. New data was collected for PTA (including TPA) and PET production. A weighted average using production amounts was calculated from the PTA production data from two plants collected from two leading producers in North America. A weighted average using production amounts was also calculated from the PET production data from two plants collected from two leading producers in North America. Data from primary sources in the early 1990's was used for DMT and PET from DMT production. The two PET technologies were weighted accordingly at 15 percent PET from DMT and 85 percent PET from PTA.

As of 2003 there were 16 PET producers and 29 PET plants in the U.S. (Reference F-2). As of 2001 there were 4 TPA/PTA producers and 6 TPA/PTA plants in the U.S. (Reference F-2). While data was collected from a small sample of plants, the PTA and PET producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American TPA/PTA and PET production. The average TPA/PTA and PET datasets were reviewed and accepted respectively by each TPA/PTA and PET data provider.

To assess the quality of the data collected for TPA/PTA, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for TPA/PTA include direct measurements, information provided by purchasing and utility records, and estimates. All data submitted for TPA/PTA represent the years 2001, 2003, and 2004 and production in the U.S.

To assess the quality of the data collected for PET from PTA, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for PET include direct measurements, information provided by purchasing and utility records, and estimates. The technology represented by the PET data is the esterification of PTA with ethylene glycol. All data submitted for PET represent the years 2001, 2003, and 2004 and production in the U.S.

Table F-8

DATA FOR THE PRODUCTION OF PET RESIN (1) (Includes PET resin, PTA, DMT, and TPA)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs (2)						
Paraxylene	521	lb		521	kg	
Ethylene glycol	322	lb		322	kg	
Acetic acid	37.2	lb		37.2	kg	
Methanol	35.2	lb		35.2	kg	
Water Consumption	64.4	gal		537	liter	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	253	kwh	2,691	558	kwh	6.27
Electricity (cogeneration)	154	cu ft (3)	172	9.59	cu meters	0.40
Natural gas	1,571	cu ft	1,760	98.1	cu meters	4.10
Bit./Sbit. Coal	18.9	lb	212	18.9	kg	0.49
Distillate oil	1.53	gal	243	12.8	liter	0.57
Residual oil	3.21	gal	551	26.8	liter	1.28
Recovered energy	61.2	thousand Btu	61.2	142	MJ	0.14
Total Process			5,568			13.0
Environmental Emissions						
Atmospheric Emissions						
Acetic Acid	0.051	lb		0.051	kg	
Aldehydes	0.094	lb		0.094	kg	
Bromine	0.079	lb		0.079	kg	
Carbon Dioxide	72.4	lb		72.4	kg	
Carbon Monoxide	5.68	lb		5.68	kg	
Methane	0.16	lb		0.16	kg	
Methyl Acetate	0.040	lb		0.040	kg	
NM Hydrocarbons	0.28	lb		0.28	kg	
Nitrogen Oxides	0.052	lb		0.052	kg	
Other Organics	0.94	lb		0.94	kg	
Particulates (unknown)	0.15	lb		0.15	kg	
Xylene	0.041	lb		0.041	kg	
Solid Wastes						
Landfilled	4.19	lb		4.19	kg	
Burned	0.31	lb		0.31	kg	
Waste-to-Energy	0.59	lb		0.59	kg	
Waterborne Wastes						
Aluminum	9.7E-07	lb		9.7E-07	kg	
Ammonia	0.11	lb		0.11	kg	
Ammonium ion	0.0013	lb		0.0013	kg	
Antimony	9.7E-07	lb		9.7E-07	kg	
BOD	0.30	lb		0.30	kg	
COD	0.76	lb		0.76	kg	
Dissolved solids	0.030	lb		0.030	kg	
Iron	9.7E-07	lb		9.7E-07	kg	
Metal ion	4.5E-06	lb		4.5E-06	kg	
Phenol	3.6E-06	lb		3.6E-06	kg	
Phosphates	5.1E-04	lb		5.1E-04	kg	
Suspended solids	0.054	lb		0.054	kg	
TOC	0.044	lb		0.044	kg	
Zinc	0.0055	lb		0.0055	kg	

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(1) PET dataset represents 15 percent from DMT technology and 85 percent from PTA technology.

(2) Methanol is produced as a coproduct of PET production from DMT. This coproduct is sent to the DMT production facilities. Due to the boundaries for this table, the recycled methanol amount is not included in the methanol raw materials.

(3) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

References: F-10 and F-18 through F-20.

Source: Franklin Associates, A Division of ERG

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APPENDIX G

GENERAL PURPOSE POLYSTYRENE (GPPS)

INTRODUCTION

This appendix discusses the manufacture of general purpose polystyrene (GPPS) resin. Examples of GPPS end-uses include food packaging, compact disc cases, and toys. Almost 6.5 billion pounds of polystyrene were produced in the U.S. and Canada in 2003 (Reference G-1). The material flow for GPPS resin is shown in Figure G-1. The total unit process energy and emissions data (cradle-to-GPPS) for GPPS are displayed in Table G-1. No fuel-related energy or emissions are included in Table G-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following processes are included in this appendix:

- Olefins Production (Pygas)
- Benzene Production
- Ethylbenzene/Styrene Production
- Mineral Oil Production
- GPPS Resin

Crude oil production, distillation, desalting and hydrotreating, natural gas production, natural gas processing, and ethylene production are discussed in Appendix B.

Olefins Production (Pygas)

The primary process used for manufacturing olefins (including pyrolysis gasoline or pygas) is the thermal cracking of saturated hydrocarbons such as ethane, propane, naphtha, and other gas oils.

Typical production of ethylene, propylene, and other coproducts begins when hydrocarbons and steam are fed to the cracking furnace. After being heated to temperatures around 1,000° Celsius, the cracked products are quenched in heat exchangers which produce high pressure steam. Fuel oil is separated from the main gas stream in a multi-stage centrifugal compressor. The main gas stream then undergoes hydrogen sulfide removal and drying. The final step involves fractional distillation of the various reaction products.

Within the hydrocracker, an offgas is produced from the raw materials entering. A portion of this offgas is used within the hydrocracker to produce steam, while the remaining portion is exported from the hydrocracker as a coproduct, as discussed below. The offgas used within the hydrocracker is shown in Table G-2 as “Internal offgas use.” This offgas is shown as a weight of natural gas and petroleum input to produce the energy, as well as the energy amount produced from those weights.

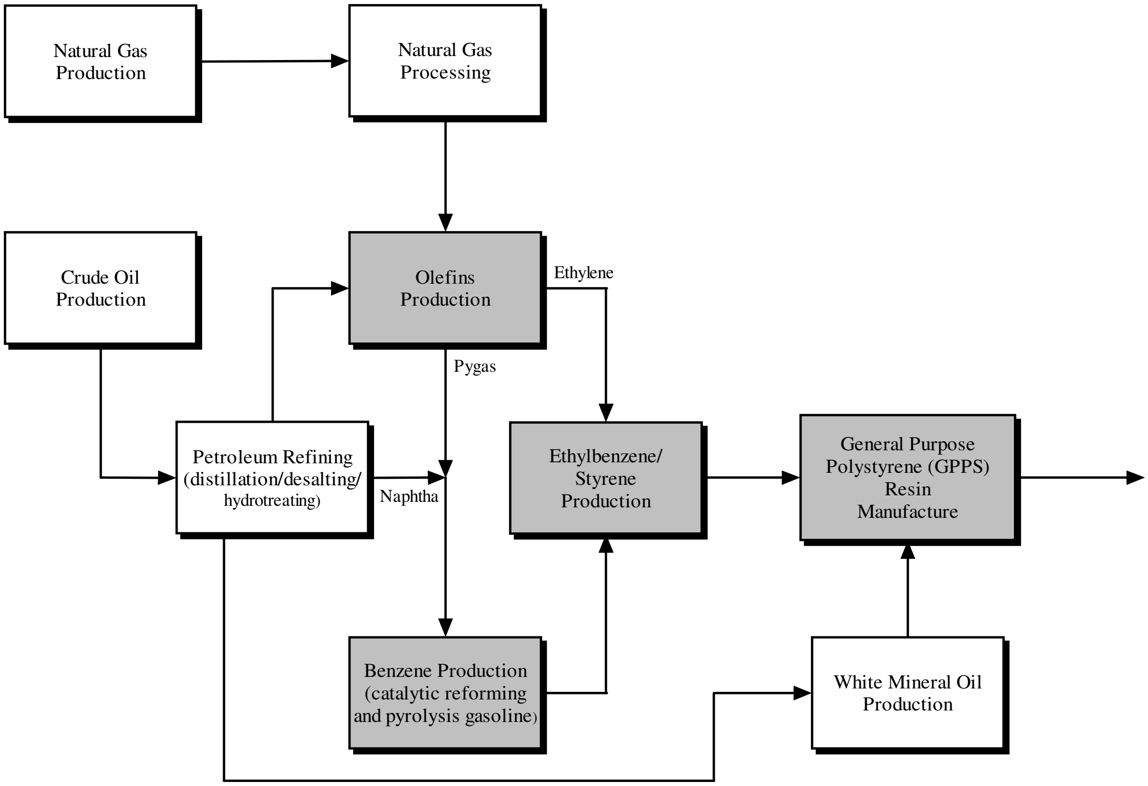

Figure G-1. Flow diagram for the production of general purpose polystyrene resin. Shaded boxes represent partial or complete data provided by manufacturers specifically for this APC analysis.

Data was collected from individual plants, and a mass allocation was used to provide an output of 1,000 pounds/kilograms of olefin product. Then a weighted average using pygas production amounts was applied to the individual olefins plant production data collected from three leading producers (8 thermal cracking units) in North America. Transportation energy for pygas was estimated using location and capacity information (References G-19 and G-20). Numerous coproduct streams are produced during this process. Fuel gas and off-gas were two of the coproducts produced that were exported to another process for fuel use. When these fuel coproducts are exported from the hydrocracker, they carry with them the allocated share of the inputs and outputs for their production. The ratio of the mass of the exported fuel over the total mass output was removed from the total inputs and outputs of the hydrocracker, and the remaining inputs and outputs are allocated over the material hydrocracker products (Equation 1).

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

where
IO = Input/Output Matrix to produce all products/coproducts
M_{EO} = Mass of Exported Offgas
M_{Total} = Mass of all Products and Coproducts (including fuels)

Table G-1

DATA FOR THE PRODUCTION OF GENERAL PURPOSE POLYSTYRENE (GPPS) RESIN

(Cradle-to-Resin)

(page 1 of 3)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	701	lb		701	kg	
Natural Gas	398	lb		398	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			8,528			19.9
Petroleum			13,158			30.6
Total Resource			21,686			50.5
Process Energy						
Electricity (grid)	230	kwh	2,448	507	kwh	5.70
Electricity (cogeneration)	116	cu ft (2)	130	7.23	cu meters	0.30
Natural gas	9,749	cu ft	10,919	609	cu meters	25.4
LPG	0.10	gal	11.3	0.87	liter	0.026
Distillate oil	0.50	gal	79.2	4.16	liter	0.18
Residual oil	5.58	gal	957	46.5	liter	2.23
Gasoline	0.11	gal	15.1	0.89	liter	0.035
Diesel	0.0033	gal	0.52	0.027	liter	0.0012
Internal Offgas use (1)						
From Oil	39.9	lb	1,105	39.9	kg	2.57
From Natural Gas	79.3	lb	2,269	79.3	kg	5.28
Recovered Energy	4.17	thousand Btu	4.17	9.69	MJ	0.0097
Total Process			17,930			41.7
Transportation Energy						
Combination truck	88.4	ton-miles		285	tonne-km	
Diesel	0.93	gal	147	7.75	liter	0.34
Rail	142	ton-miles		457	tonne-km	
Diesel	0.35	gal	55.9	2.94	liter	0.13
Barge	425	ton-miles		1,368	tonne-km	
Diesel	0.34	gal	54.0	2.84	liter	0.13
Residual oil	1.13	gal	194	9.43	liter	0.45
Ocean freighter	1,170	ton-miles		3,764	tonne-km	
Diesel	0.22	gal	35.3	1.85	liter	0.082
Residual	2.00	gal	343	16.7	liter	0.80
Pipeline-natural gas	238	ton-miles		765	tonne-km	
Natural gas	164	cu ft	184	10.2	cu meter	0.43
Pipeline-petroleum products	242	ton-miles		778	tonne-km	
Electricity	5.27	kwh	54.0	11.6	kwh	0.13
Total Transportation			1,067			2.48

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table G-1

DATA FOR THE PRODUCTION
OF GENERAL PURPOSE POLYSTYRENE (GPPS) RESIN
(Cradle-to-Resin)
(page 2 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Ammonia	0.0026	lb	0.0026	kg
Antimony	1.5E-06	lb	1.5E-06	kg
Arsenic	1.9E-07	lb	1.9E-07	kg
Benzene	0.047	lb	0.047	kg
Carbon Dioxide - Fossil	330	lb	330	kg
Carbon Monoxide	0.61	lb	0.61	kg
Carbon Tetrachloride	9.9E-07	lb	9.9E-07	kg
CFC 13 (Methane, trichlorofluoro-)	1.6E-05	lb	1.6E-05	kg
Chlorine	1.3E-04	lb	1.3E-04	kg
Chromium	4.9E-07	lb	4.9E-07	kg
Ethylbenzene	0.0055	lb	0.0055	kg
Ethylene Dibromide	3.1E-06	lb	3.1E-06	kg
HCFC-22	0.0010	lb	0.0010	kg
Hydrogen	0.0026	lb	0.0026	kg
Hydrogen Chloride	5.5E-07	lb	5.5E-07	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.49	lb	0.49	kg
Methane	6.48	lb	6.48	kg
Methyl Ethyl Ketone	2.6E-04	lb	2.6E-04	kg
Nickel	4.2E-06	lb	4.2E-06	kg
Nitrogen Oxides	0.50	lb	0.50	kg
Non-Methane Hydrocarbons	0.19	lb	0.19	kg
Other Organics	0.011	lb	0.011	kg
Particulates (PM10)	0.079	lb	0.079	kg
Particulates (PM2.5)	0.025	lb	0.025	kg
Particulates (unspecified)	0.054	lb	0.054	kg
Polyaromatic Hydrocarbons (total)	4.1E-05	lb	4.1E-05	kg
Sulfur Dioxide	1.08	lb	1.08	kg
Sulfur Oxides	0.35	lb	0.35	kg
Toluene	0.071	lb	0.071	kg
VOC	0.38	lb	0.38	kg
Xylene	0.041	lb	0.041	kg
Solid Wastes				
Landfilled	38.7	lb	38.7	kg
Burned	3.43	lb	3.43	kg
Waste-to-Energy	1.55	lb	1.55	kg
Waterborne Wastes				
m-Xylene	8.2E-06	lb	8.2E-06	kg
1-Methylfluorene	1.3E-08	lb	1.3E-08	kg
2,4-Dimethylphenol	8.0E-06	lb	8.0E-06	kg
2-Hexanone	1.9E-06	lb	1.9E-06	kg
2-Methylnaphthalene	4.3E-06	lb	4.3E-06	kg
4-Methyl-2-Pentanone	4.9E-07	lb	4.9E-07	kg
Acetone	1.2E-06	lb	1.2E-06	kg
Acid (benzoic)	2.9E-04	lb	2.9E-04	kg
Acid (hexanoic)	6.0E-05	lb	6.0E-05	kg
Alkylated benzenes	5.4E-05	lb	5.4E-05	kg
Alkylated fluorenes	3.2E-06	lb	3.2E-06	kg
Alkylated naphthalenes	8.9E-07	lb	8.9E-07	kg
Alkylated phenanthrenes	3.7E-07	lb	3.7E-07	kg
Aluminum	0.027	lb	0.027	kg
Ammonia	0.015	lb	0.015	kg
Antimony	1.7E-05	lb	1.7E-05	kg
Arsenic	5.7E-05	lb	5.7E-05	kg
Barium	0.36	lb	0.36	kg
Benzene	3.2E-04	lb	3.2E-04	kg
Beryllium	3.6E-06	lb	3.6E-06	kg
BOD	0.42	lb	0.42	kg
Boron	8.9E-04	lb	8.9E-04	kg
Bromide	0.037	lb	0.037	kg
Cadmium	8.8E-06	lb	8.8E-06	kg
Calcium	0.61	lb	0.61	kg
Chlorides	7.51	lb	7.51	kg
Chromium (hexavalent)	2.3E-07	lb	2.3E-07	kg
Chromium (unspecified)	7.3E-04	lb	7.3E-04	kg

Table G-1

DATA FOR THE PRODUCTION OF GENERAL PURPOSE POLYSTYRENE (GPPS) RESIN
(Cradle-to-Resin)
(page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Cobalt	6.3E-06	lb	6.3E-06	kg
COD	1.07	lb	1.07	kg
Copper	7.8E-05	lb	7.8E-05	kg
Cyanide	1.0E-06	lb	1.0E-06	kg
Dibenzofuran	2.2E-08	lb	2.2E-08	kg
Dibenzothiophene	1.8E-08	lb	1.8E-08	kg
Dissolved Solids	8.86	lb	8.86	kg
Ethylbenzene	0.0010	lb	0.0010	kg
Fluorene	1.5E-06	lb	1.5E-06	kg
Hydrocarbons	1.0E-05	lb	1.0E-05	kg
Iron	0.050	lb	0.050	kg
Lead	1.6E-04	lb	1.6E-04	kg
Lead 210	3.0E-14	lb	3.0E-14	kg
Lithium	0.072	lb	0.072	kg
Magnesium	0.12	lb	0.12	kg
Manganese	1.8E-04	lb	1.8E-04	kg
Mercury	3.4E-07	lb	3.4E-07	kg
Methyl Chloride	4.7E-09	lb	4.7E-09	kg
Methyl Ethyl Ketone	9.5E-09	lb	9.5E-09	kg
Molybdenum	6.6E-06	lb	6.6E-06	kg
Naphthalene	5.2E-06	lb	5.2E-06	kg
n-Decane	8.3E-06	lb	8.3E-06	kg
n-Docosane	1.3E-07	lb	1.3E-07	kg
n-Dodecane	1.6E-05	lb	1.6E-05	kg
n-Eicosane	4.3E-06	lb	4.3E-06	kg
n-Hexacosane	7.8E-08	lb	7.8E-08	kg
n-Hexadecane	1.7E-05	lb	1.7E-05	kg
Nickel	7.8E-05	lb	7.8E-05	kg
n-Octadecane	4.3E-06	lb	4.3E-06	kg
p -Xylene	3.0E-06	lb	3.0E-06	kg
o -Xylene	3.0E-06	lb	3.0E-06	kg
o-Cresol	8.2E-06	lb	8.2E-06	kg
Oil	0.027	lb	0.027	kg
p-Cresol	8.9E-06	lb	8.9E-06	kg
p-Cymene	1.2E-08	lb	1.2E-08	kg
Pentamethylbenzene	8.8E-09	lb	8.8E-09	kg
Phenanthrene	2.3E-07	lb	2.3E-07	kg
Phenol/ Phenolic Compounds	8.1E-04	lb	8.1E-04	kg
Phosphates	0.0010	lb	0.0010	kg
Tetradecane	6.6E-06	lb	6.6E-06	kg
Radium 226	1.0E-11	lb	1.0E-11	kg
Radium 228	5.3E-14	lb	5.3E-14	kg
Selenium	4.4E-06	lb	4.4E-06	kg
Silver	3.8E-04	lb	3.8E-04	kg
Sodium	1.78	lb	1.78	kg
Strontium	0.016	lb	0.016	kg
Styrene	0.0010	lb	0.0010	kg
Sulfates	0.013	lb	0.013	kg
Sulfides	9.2E-04	lb	9.2E-04	kg
Sulfur	7.0E-04	lb	7.0E-04	kg
Surfactants	1.5E-04	lb	1.5E-04	kg
Suspended Solids	2.98	lb	2.98	kg
Thallium	3.5E-06	lb	3.5E-06	kg
Tin	6.6E-05	lb	6.6E-05	kg
Titanium	2.6E-04	lb	2.6E-04	kg
TOC	5.6E-04	lb	5.6E-04	kg
Toluene	3.5E-04	lb	3.5E-04	kg
Total biphenyls	3.5E-06	lb	3.5E-06	kg
Total dibenzothiophenes	1.1E-08	lb	1.1E-08	kg
Vanadium	4.7E-05	lb	4.7E-05	kg
Xylene, unspecified	1.4E-04	lb	1.4E-04	kg
Yttrium	1.9E-06	lb	1.9E-06	kg
Zinc	6.2E-04	lb	6.2E-04	kg

References: Tables B-2 through B-6 and G-2 through G-6.

Source: Franklin Associates, A Division of ERG models

Table G-2

DATA FOR THE PRODUCTION OF PYGAS

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs (1)							
Refined Petroleum Products	419	lb			419	kg	
Processed Natural Gas	584	lb			584	kg	
Water Consumption	93.5	gal			780	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	52.6	kwh		560	116	kwh	1.30
Electricity (cogeneration)	127	cu ft	(3)	142	7.93	cu meters	0.33
Natural Gas	1,544	cu ft		1,730	96.4	cu meters	4.03
Gasoline	0.0022	gal		0.31	0.018	liter	7.3E-04
Diesel	0.0019	gal		0.30	0.016	liter	7.1E-04
Internal Offgas use (2)							
From Oil	75.2	lb		2,127	75.2	kg	4.95
From Natural Gas	104	lb		2,937	104	kg	6.84
Recovered Energy	2.50	thousand Btu		2.50	5.82	MJ	0.0058
Total Process				7,494			17.4
Transportation Energy							
Rail	115	ton-miles			370	tonne-km	
Diesel	0.29	gal		45.3	2.38	liter	0.11
Pipeline-Petroleum Products	1.55	ton-miles			4.99	tonne-km	
Electricity	0.034	kwh		0.35	0.074	kwh	8.0E-04
Total Transportation				45.6			0.11
Environmental Emissions							
Atmospheric Emissions - Process							
Carbon Monoxide	0.0010	lb	(4)		0.0010	kg	
Chlorine	1.0E-04	lb	(4)		1.0E-04	kg	
HCFC-022	1.0E-06	lb	(4)		1.0E-06	kg	
Hydrogen Chloride	1.0E-06	lb	(4)		1.0E-06	kg	
Hydrogen	0.0052	lb			0.0052	kg	
Hydrocarbons (NM)	0.11	lb			0.11	kg	
Methane	0.0010	lb	(4)		0.0010	kg	
Other Organics	0.0010	lb	(4)		0.0010	kg	
Particulates (unspecified)	0.010	lb			0.010	kg	
Particulates (PM10)	0.10	lb	(4)		0.10	kg	
Sulfur Oxides	0.0044	lb			0.0044	kg	
VOC	0.010	lb	(4)		0.010	kg	
Atmospheric Emissions - Fuel-Related (5)							
Carbon Dioxide (fossil)	661	lb			661	kg	
Carbon Monoxide	0.29	lb			0.29	kg	
Nitrogen Oxides	0.43	lb			0.43	kg	
PM 2.5	0.009	lb			0.009	kg	
Sulfur Oxides	0.068	lb			0.068	kg	
Solid Wastes							
Landfilled	0.36	lb			0.36	kg	
Burned	6.89	lb			6.89	kg	
Waste-to-Energy	0.0047	lb			0.0047	kg	
Waterborne Wastes							
Acetone	1.0E-08	lb	(4)		1.0E-08	kg	
Benzene	1.0E-05	lb	(4)		1.0E-05	kg	
BOD	3.5E-04	lb			3.5E-04	kg	
COD	0.010	lb	(4)		0.010	kg	
Ethylbenzene	1.0E-05	lb	(4)		1.0E-05	kg	
Naphthalene	1.0E-08	lb	(4)		1.0E-08	kg	
Phenol	0.0010	lb	(4)		0.0010	kg	
Styrene	1.0E-06	lb	(4)		1.0E-06	kg	
Suspended Solids	0.0028	lb			0.0028	kg	
Toluene	1.0E-04	lb	(4)		1.0E-04	kg	
Total Organic Carbon	0.0010	lb	(4)		0.0010	kg	
Xylene	1.0E-06	lb	(4)		1.0E-06	kg	

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(1) Specific raw 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.

(3) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(4) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(5) These fuel-related emissions were provided by the plants. These take into account the combustion of the offgas as well as the natural gas.

References: G-5, G-6, and G-19 through G-21.

Source: Franklin Associates, A Division of ERG

No energy credit is applied for the exported fuels, since both the inputs and outputs for the exported fuels have been removed from the data set. Table G-2 shows the averaged energy and emissions data for the production of pyrolysis gasoline.

As of 2003, there were 16 olefin producers and at least 29 olefin plants in the U.S. (Reference G-20). While data was collected from a relatively small sample of plants, the olefins producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American olefins production. All data collected were individually reviewed by the data providers.

To assess the quality of the data collected for olefins, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for olefins include direct measurements, information provided by purchasing and utility records, and estimates. The standard production technology for olefins is the steam cracking of hydrocarbons (including natural gas liquids and petroleum liquids). The data in this module represent steam cracking of natural gas and petroleum. All data submitted for olefins represent the year 2003 and U.S. and Canada production.

Benzene Production

Benzene is the most widely used aromatic petrochemical raw material. The two major sources of benzene are catalytic reformate and pyrolysis gasoline (Reference G-2). Additional benzene is produced by the dealkylation of the toluene.

In the reforming process, naphtha is fed through a catalyst bed at elevated temperatures and pressures. The most common type of reforming process is platforming, in which a platinum-containing catalyst is used. Products obtained from the platforming process include aromatic compounds (benzene, toluene, xylene), hydrogen, light gas, and liquefied petroleum gas. The aromatics content of the reformate varies and is normally less than 45 percent. The reformate from the platforming process undergoes solvent extraction and fractional distillation to produce pure benzene, toluene, and other coproducts.

Pyrolysis gasoline is a byproduct of the steam cracking of hydrocarbons for the production of ethylene and propylene. Raw pyrolysis gas is composed of a mixture of C_5 to C_8 hydrocarbons, including several aromatic compounds. To separate the aromatics from the resulting mixture, a very polar solvent (commonly an alcohol) is used to dissolve the aromatic components. The aromatics can then be separated from the solvent using fractional distillation. The solvent is recovered and re-used.

Table G-3 represents the energy requirements and environmental emissions for producing benzene. Only catalytic reforming and pyrolysis gasoline are considered as the source of benzene in this analysis. These sources account for 70 percent of the world production of benzene (Reference G-3). It is estimated that one-third of this production is from pyrolysis gasoline and two-thirds are produced from catalytic reforming (Reference G-4). The collected datasets were weighted using these fractions.

Numerous aromatic coproduct streams are produced during this process. Fuel gas and off-gas were two of the coproducts produced that were exported to another process for fuel use. When these fuel coproducts are exported from the aromatics separation process, they carry with them the allocated share of the inputs and outputs for their production. The ratio of the mass of the exported fuel over the total mass output was removed from the total inputs and outputs, and the remaining inputs and outputs are allocated over the material aromatics products (Equation 1).

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

where
IO = Input/Output Matrix to produce all products/coproducts
M_{EO} = Mass of Exported Offgas
M_{Total} = Mass of all Products and Coproducts (including fuels)

No energy credit is applied for the exported fuels, since both the inputs and outputs for the exported fuels have been removed from the data set. Table G-3 shows the averaged energy and emissions data for the production of benzene.

As of 2002 there were 22 benzene producers and 38 benzene plants in the U.S. for the three standard technologies (Reference G-19). The benzene data collected for this module represent 1 producer and 1 plant in the U.S. While data was collected from a small sample of plants, the benzene producer who provided data for this module verified that the characteristics of their plant is representative of the extraction of benzene from pyrolysis gasoline for North American benzene production. The average dataset was reviewed and accepted by the benzene data provider.

One of the three datasets was collected for this project and represents 2003 data, while the other two datasets comes from 1992. The 2003 data were collected from direct measurements and engineering estimates. The collection methods for the 1992 data are unknown.

Table G-3

DATA FOR THE PRODUCTION OF BENZENE

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Naphtha	667	lb			667	kg	
Pygas from Hydrocracker	335	lb			335	kg	
Water Consumption	0.75	gal			6.26	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	7.22	kwh		74.3	15.9	kwh	0.17
Electricity (cogeneration)	28.8	cu ft	(2)	32.3	1.80	cu meters	0.075
Natural gas	631	cu ft		707	39.4	cu meters	1.65
Distillate oil	0.40	gal		63.5	3.34	liter	0.15
Residual oil	3.87	gal		664	32.3	liter	1.55
Internal Offgas use (1)							
From Oil	16.0	lb		400.6	16.0	kg	0.93
From Natural Gas	22.1	lb		553.4	22.1	kg	1.29
Total Process				2,495			3.23
Transportation Energy							
Barge	57.5	ton-miles			185	tonne-km	
Diesel	0.046	gal		7.30	0.15	gal	23.5
Residual oil	0.15	gal		26.2	0.49	gal	84.5
Pipeline-petroleum products	0.50	ton-miles			1.61	tonne-km	
Electricity	0.011	kwh		0.11	0.024	kwh	2.6E-04
Total Transportation				33.7			108
Environmental Emissions							
Atmospheric Emissions							
Chlorine	1.0E-04	lb	(3)		1.0E-04	kg	
Carbon Dioxide	45.2	lb			45.2	kg	
Carbon Monoxide	0.010	lb	(3)		0.010	kg	
NM Hydrocarbons	0.010	lb	(3)		0.010	kg	
Nitrogen Oxides	0.062	lb			0.062	kg	
Hydrogen	1.0E-06	lb	(3)		1.0E-06	kg	
Particulates (unknown)	0.019	lb			0.019	kg	
PM2.5	0.010	lb	(3)		0.010	kg	
PM10	0.0010	lb	(3)		0.0010	kg	
Sulfur Oxides	0.44	lb			0.44	kg	
Solid Wastes							
Landfilled	0.43	lb			0.43	kg	
Burned	0.051	lb			0.051	kg	
Waterborne Wastes							
Benzene	1.0E-06	lb	(3)		1.0E-06	kg	
BOD	0.47	lb			0.47	kg	
COD	1.08	lb			1.08	kg	
Dissolved solids	0.11	lb			0.11	kg	
Oil	0.018	lb			0.018	kg	
Sulfides	0.0010	lb	(3)		0.0010	kg	
Suspended Solids	0.0010	lb	(3)		0.0010	kg	
TOC	1.0E-05	lb	(3)		1.0E-05	kg	

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(3) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

References: G-5 through G-9

Source: Franklin Associates, A Division of ERG

Ethylbenzene/Styrene Production

The production of styrene monomer is accomplished through a series of processes. The first is the production of ethylbenzene by the alkylation of benzene with ethylene. In this process, benzene initially passes through a drying column. From the drying column, the benzene and ethylene are mixed in a reactor with a suitable catalyst. This reaction is exothermic and occurs at relatively low pressures and temperatures. Unreacted benzene is removed and recycled back to the process. The ethylbenzene is then separated from the solution. The heavy bottoms, tars, and vent gases are burned while the solution is recycled back to the reactor.

Styrene is produced by dehydrogenation of ethylbenzene. The ethylbenzene is mixed with steam, then allowed to come in contact with a catalyst in a reactor. This reaction is carried out at high temperature under vacuum. The heat is recovered from this reaction, and the hydrocarbon solution is sent to a series of fractionation units. The first separation removes the small amount (4 to 6 percent) of toluene and benzene produced by cracking. This toluene/benzene stream is typically sent back to the benzene plant. The second separation removes unreacted ethylbenzene and recycles it back into the system. Purified styrene monomer is recovered in the third and final phase. Bottoms or tar residue is removed from this third phase (Reference G-10).

Table G-4 displays the energy requirements and environmental emissions for the production of styrene including the production of ethylbenzene. Two of the three ethylbenzene/styrene datasets were collected for this project and represents 2002-2003 data, while the other dataset comes from 1993. The 2003 data were collected from direct measurements, purchasing/utility records, and engineering estimates. The collection methods for the 1993 data are unknown. Various coproduct streams are produced during this process. A mass basis was used to partition the credit for these coproducts.

As of 2001 there were 8 styrene producers and 8 styrene plants in the U.S. (Reference G-5). The styrene data collected for this module represent 2 producers and 2 plants in the U.S. While data was collected from a small sample of plants, the styrene producers who provided data for this module verified that the characteristics of their plants are representative of North American styrene production. The average dataset was reviewed and accepted by the styrene data providers.

Table G-4

DATA FOR THE PRODUCTION OF ETHYLBENZENE/STYRENE

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Ethylene	293	lb			293	kg	
Benzene	783	lb			783	kg	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	74.2	kwh		764	164	kwh	1.78
Electricity (cogeneration)	0.66	cu ft	(1)	0.74	0.041	cu meters	0.0017
Natural gas	6,835	cu ft		7,655	427	cu meters	17.8
Total Process				8,420			19.6
Transportation Energy							
To Polystyrene product							
Combination truck	75.5	ton-miles			243	tonne-km	
Diesel	0.79	gal		126	6.61	liter	0.29
Rail	103	ton-miles			330	tonne-km	
Diesel	0.25	gal		40.4	2.12	liter	0.094
Barge	326	ton-miles			1,049	tonne-km	
Diesel	0.26	gal		41.4	2.18	liter	0.096
Residual oil	0.87	gal		149	7.24	liter	0.35
Ocean freighter	78.0	ton-miles			251	tonne-km	
Diesel	0.015	gal		2.35	0.12	liter	0.0055
Residual	0.13	gal		22.9	1.11	liter	0.053
Total Transportation				382			0.89
To ABS product							
Rail	59.2	ton-miles			191	tonne-km	
Diesel	0.15	gal		23.3	1.23	liter	0.054
Barge	398	ton-miles			1,281	tonne-km	
Diesel	0.32	gal		50.6	2.66	liter	0.12
Residual oil	1.06	gal		182	8.83	liter	0.42
Ocean freighter	62.7	ton-miles			202	tonne-km	
Diesel	0.012	gal		1.89	0.10	liter	0.0044
Residual	0.11	gal		18.4	0.89	liter	0.043
Total Transportation				276			0.64
Environmental Emissions							
Atmospheric Emissions							
Carbon Monoxide	0.27	lb			0.27	kg	
Carbon Dioxide	261	lb			261	kg	
NM Hydrocarbons	0.010	lb	(2)		0.010	kg	
Nitrogen Oxides	0.10	lb	(2)		0.10	kg	
Particulates (unknown)	0.010	lb	(2)		0.010	kg	
Sulfur Oxides	1.0E-04	lb	(2)		1.0E-04	kg	
VOC	0.0093	lb			0.0093	kg	
Solid Wastes							
Landfilled	1.61	lb			1.61	kg	
Burned	0.44	lb			0.44	kg	
Waterborne Wastes							
Ethylbenzene	0.0010	lb	(2)		0.0010	kg	
Styrene	0.0010	lb	(2)		0.0010	kg	
Suspended Solids	0.010	lb	(2)		0.010	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

References: G-11 through G-13

Source: Franklin Associates, A Division of ERG

Mineral Oil Production

Mineral oils are mixtures of highly refined paraffinic and naphthenic liquid hydrocarbons and have boiling points greater than 200° Celsius (Reference G-14). The initial distillation of crude oil is used to remove lighter petroleum fractions, such as gasoline and naphtha, and the remaining fractions consist of raw materials for fuel oil, coke, lubrication grease, and asphalts. This residue is processed through a vacuum distillation column to isolate the raw materials for lubricating oil production.

Lubricating oil production includes hydrotreating, deasphalting, and dewaxing processes that eliminate components such as multiple-ring aromatics, asphalt-like compounds, and straight-chain paraffins. The extensive refining requirements for mineral oil production result in high energy requirements in comparison to other refinery products. However, mineral oil (and other components of the lubricating oil category) represent less than one percent of total refinery output; thus, while they are energy intensive, they represent a small share of total refinery energy.

Mineral oil is used in plastics, such as polystyrene, to improve and control the melt flow rate of the finished polymer (Reference G-14). The energy and environmental burdens in Table G-5 apply to the production of mineral oil.

General Purpose Polystyrene (GPPS) Resin Production

General-purpose polystyrene (GPPS) is produced by dispensing styrene in water in a reactor and polymerizing in the presence of initiators and suspending agents. Mass polymerization is the most common polymerization process for GPPS in the United States.

Mass polymerization, also known as bulk polymerization, is one of the simplest methods of polymerization. It is often used in the polymerization of step-growth polymers. During step-growth polymerization, the functional sites of monomers react, liberate a small molecule such as water, and repeat the reaction to produce longer and longer polymer chains. Mass polymerization does not suspend the reactants in a solution such as water or organic solvents. The absence of a reaction solution makes heat control difficult and, if not monitored carefully, a mass polymerization reaction can progress too rapidly and overheating or hot spots can occur in the reaction vessel. However, since water or organic solvents are not used, there is a lower chance for contamination of the product (References G-2 and G-17).

After the reactor and contents are cooled, the beads are dewatered and dried. The wastewater is sent to an effluent treatment facility. The dried beads are screened into different sizes and the GPPS resin is packed into containers for shipment to molders.

Data for the production of GPPS resin using mass polymerization were provided by four leading producers (6 plants) in North America to Franklin Associates under contract to Plastics Division of the American Chemistry Council (ACC). The energy requirements and environmental emissions for the production of GPPS resin are shown in Table G-6. Scrap is produced as a coproduct during this process. A mass basis was used to partition the credit for scrap.

As of 2002 there were 12 PS producers and 24 PS plants in the U.S. (Reference G-5). These plants produce all types of polystyrene; it is unknown how many produce GPPS. While data was collected from a small sample of plants, the GPPS producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American GPPS production. The average dataset was reviewed and accepted by all GPPS data providers.

To assess the quality of the data collected for GPPS, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for GPPS include direct measurements, information provided by purchasing and utility records, and estimates. The technology represented by the GPPS data represents polymerization by mass suspension. All data submitted for GPPS ranges from 2000 through 2003 and represents U.S. production.

Table G-5

DATA FOR THE PRODUCTION OF MINERAL OIL FROM REFINED OIL

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Refined oil	1,000	lb		1,000	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	188	kwh	1,935	414	kwh	4.50
Natural gas	1,195	cu ft	1,338	74.6	cu meters	3.12
LPG	0.93	gal	101	7.76	liter	0.23
Residual oil	21.8	gal	3,741	182	liter	8.71
Total Process			7,115			16.6
Transportation Energy						
Combination truck	275	ton-miles		885	tonne-km	
Diesel	2.89	gal	459	24.1	liter	1.07
Rail	275	ton-miles		885	tonne-km	
Diesel	0.68	gal	108	5.69	liter	0.25
Total Transportation			567			1.32
Environmental Emissions						
Atmospheric Emissions						
Methylethylketone (MEK)	0.10	lb		0.10	kg	
VOC	0.10	lb		0.10	kg	
Waterborne Wastes.						
Chromium (unspecified)	0.0010	lb		0.0010	kg	
Chromium (Hexavalent)	8.7E-05	lb		8.7E-05	kg	
Phenolic Compounds	9.0E-04	lb		9.0E-04	kg	

References: G-6, G-8, and G-15

Source: Franklin Associates, A Division of ERG

Table G-6

DATA FOR THE PRODUCTION OF GENERAL PURPOSE POLYSTYRENE (GPPS)

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Styrene	999	lb			999	kg	
Mineral oil	2.57	lb			2.57	kg	
Water Consumption	47.4	gal			395	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	52.2	kwh		537	115	kwh	1.25
Natural gas	321	cu ft		360	20.0	cu meter	0.84
Total Process				897			2.09
Environmental Emissions							
Atmospheric Emissions							
Carbon Monoxide	0.019	lb			0.019	kg	
HCFC-022	0.001	lb	(1)		0.001	kg	
Hydrocarbons (NM)	0.120	lb			0.120	kg	
Nitrogen Oxides	0.043	lb			0.043	kg	
Other Organics	0.01	lb	(1)		0.010	kg	
Particulates (unknown)	0.024	lb			0.024	kg	
Sulfur Oxides	3.3E-04	lb			0.000	kg	
Solid Wastes							
Landfilled	0.63	lb			0.63	kg	
Burned	0.017	lb			0.02	kg	
Waste-to-Energy	1.54	lb			1.54	kg	
Waterborne Wastes							
Ammonia	1.E-04	lb	(1)		5.E-04	kg	
BOD	1.E-04	lb	(1)		1.E-04	kg	
Chromium	1.E-05	lb	(1)		5.E-05	kg	
Cyanide	1.E-06	lb	(1)		1.E-06	kg	
Dissolved solids	1	lb	(1)		1	kg	
Hydrocarbons	1.E-05	lb	(1)		1.E-05	kg	
Iron	1.E-05	lb	(1)		1.E-05	kg	
Lead	1.E-05	lb	(1)		5.E-05	kg	
Nickel	1.E-05	lb	(1)		5.E-05	kg	
Oil	1.E-04	lb	(1)		1.E-04	kg	
Phenol	1.E-06	lb	(1)		1.E-06	kg	
Phosphates	0.001	lb	(1)		0.001	kg	
Suspended Solids	1.E-04	lb	(1)		5.E-04	kg	
Zinc	2.E-05	lb			5.E-05	kg	

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(1) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

References: G-13 and G-18

Source: Franklin Associates, A Division of ERG

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APPENDIX H

HIGH-IMPACT POLYSTYRENE (HIPS)

INTRODUCTION

This appendix discusses the manufacture of high-impact polystyrene (HIPS) resin. Examples of HIPS end-uses are flatware and medical products. Almost 6.5 billion pounds of polystyrene in general were produced in the U.S. and Canada in 2003 (Reference H-1). The material flow for HIPS resin is shown in Figure H-1. The total unit process energy and emissions data (cradle-to-HIPS) for HIPS are displayed in Table H-1. No fuel-related energy or emissions are included in Table H-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following processes are included in this appendix:

- Butadiene Production
- Polybutadiene Production
- HIPS Resin

Crude oil production, distillation, desalting and hydrotreating, natural gas production, natural gas processing, and ethylene production are discussed in Appendix B. Pygas production, benzene production, and ethylbenzene/styrene production are discussed in Appendix G.

Butadiene Production

Commercial routes to production of butadiene are dehydrogenation of n-butane and n-butenes, and formation as a by-product during the manufacture of olefins. As of 2002, almost all butadiene is produced as an ethylene steam-cracking coproduct (Reference H-2).

Typical production of ethylene, propylene, and other coproducts begins when hydrocarbons and steam are fed to the cracking furnace. After being heated to temperatures around 1,000° Celsius, the cracked products are quenched in heat exchangers which produce high pressure steam. Fuel oil is separated from the main gas stream in a multi-stage centrifugal compressor. The main gas stream then undergoes hydrogen sulfide removal and drying. The final step involves fractional distillation of the various reaction products.

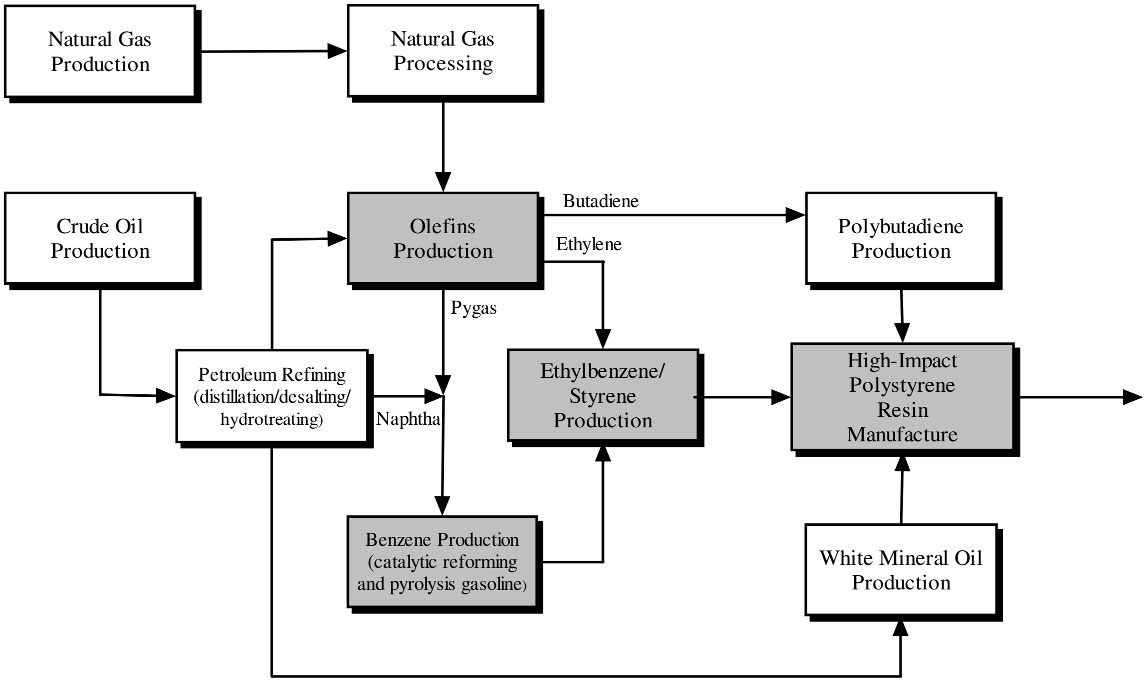

Figure H-1. Flow diagram for the production of high-impact polystyrene resin. Shaded boxes represent partial or complete data provided by manufacturers specifically for this APC analysis.

Within the hydrocracker, an offgas is produced from the raw materials entering. A portion of this offgas is used within the hydrocracker to produce steam, while the remaining portion is exported from the hydrocracker as a coproduct, as discussed below. The offgas used within the hydrocracker is shown in Table H-2 as “Internal offgas use.” This offgas is shown as a weight of natural gas and petroleum input to produce the energy, as well as the energy amount produced from those weights.

Data was collected from individual plants, and a mass allocation was used to provide an output of 1,000 pounds/kilograms of olefin product. Then a weighted average using butadiene production amounts was applied to the individual olefins plant production data collected from three leading producers (3 thermal cracking units) in North America. Transportation amounts for butadiene were estimated (References H-2 and H-4). Numerous coproduct streams are produced during this process. Fuel gas and off-gas were two of the coproducts produced that were exported to another process for fuel use. When these fuel coproducts are exported from the hydrocracker, they carry with them the allocated share of the inputs and outputs for their production. The ratio of the mass of the exported fuel over the total mass output was removed from the total inputs and outputs of the hydrocracker, and the remaining inputs and outputs are allocated over the material hydrocracker products (Equation 1).

Table H-1

DATA FOR THE PRODUCTION
OF HIGH-IMPACT POLYSTYRENE (HIPS) RESIN
(Cradle-to-Resin)
(page 1 of 3)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	697	lb		697	kg	
Natural Gas	415	lb		415	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			8,897			20.7
Petroleum			13,074			30.4
Total Resource			21,971			51.1
Process Energy						
Electricity (grid)	235	kwh	2,496	517	kwh	5.81
Electricity (cogeneration)	159	cu ft (2)	178	9.92	cu meters	0.41
Natural gas	9,522	cu ft	10,664	594	cu meters	24.8
LPG	0.12	gal	12.8	0.99	liter	0.030
Distillate oil	0.48	gal	76.6	4.02	liter	0.18
Residual oil	5.72	gal	982	47.8	liter	2.29
Gasoline	0.11	gal	15.4	0.90	liter	0.036
Diesel	0.0033	gal	0.52	0.027	liter	0.0012
Internal Offgas use (1)						
From Oil	42.7	lb	1,184	42.7	kg	2.76
From Natural Gas	83.9	lb	2,390	83.9	kg	5.56
Recovered Energy	4.14	thousand Btu	4.14	9.63	MJ	0.0096
Total Process			17,995			41.9
Transportation Energy						
Combination truck	123	ton-miles		396	tonne-km	
Diesel	1.29	gal	205	10.8	liter	0.48
Rail	146	ton-miles		470	tonne-km	
Diesel	0.36	gal	57.5	3.02	liter	0.13
Barge	430	ton-miles		1,383	tonne-km	
Diesel	0.34	gal	54.6	2.87	liter	0.13
Residual oil	1.14	gal	196	9.54	liter	0.46
Ocean freighter	1,162	ton-miles		3,741	tonne-km	
Diesel	0.22	gal	35.1	1.84	liter	0.082
Residual	1.99	gal	341	16.6	liter	0.79
Pipeline-natural gas	249	ton-miles		800	tonne-km	
Natural gas	172	cu ft	192	10.7	cu meter	0.45
Pipeline-petroleum products	243	ton-miles		782	tonne-km	
Electricity	5.30	kwh	54.2	11.7	kwh	0.13
Total Transportation			1,136			2.64

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table H-1

DATA FOR THE PRODUCTION
OF HIGH-IMPACT POLYSTYRENE (HIPS) RESIN
(Cradle-to-Resin)
(page 2 of 3)

	English units (Basis: 1,000 lb)	SI units (Basis: 1,000 kg)
Environmental Emissions		
Atmospheric Emissions		
Acid (unknown)	1.0E-06 lb	1.0E-06 kg
Ammonia	0.0026 lb	0.0026 kg
Antimony	1.5E-06 lb	1.5E-06 kg
Arsenic	1.9E-07 lb	1.9E-07 kg
Benzene	0.049 lb	0.049 kg
Carbon Dioxide - Fossil	313 lb	313 kg
Carbon Monoxide	0.58 lb	0.58 kg
Carbon Tetrachloride	9.9E-07 lb	9.9E-07 kg
CFC 13 (Methane, trichlorofluoro-)	1.6E-05 lb	1.6E-05 kg
Chlorine	1.3E-04 lb	1.3E-04 kg
Chromium	4.9E-07 lb	4.9E-07 kg
Ethylbenzene	0.0057 lb	0.0057 kg
Ethylene Dibromide	3.1E-06 lb	3.1E-06 kg
HCFC-22	0.0010 lb	0.0010 kg
Hydrogen	0.0024 lb	0.0024 kg
Hydrogen Chloride	5.2E-07 lb	5.2E-07 kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.49 lb	0.49 kg
Methane	6.58 lb	6.58 kg
Methyl Ethyl Ketone	0.0018 lb	0.0018 kg
Nickel	4.2E-06 lb	4.2E-06 kg
Nitrogen Oxides	0.49 lb	0.49 kg
Non-Methane Hydrocarbons	0.93 lb	0.93 kg
Other Organics	0.010 lb	0.010 kg
Particulates (PM10)	0.092 lb	0.092 kg
Particulates (PM2.5)	0.024 lb	0.024 kg
Particulates (unspecified)	0.044 lb	0.044 kg
Polyaromatic Hydrocarbons (total)	4.1E-05 lb	4.1E-05 kg
Sulfur Dioxide	1.12 lb	1.12 kg
Sulfur Oxides	0.33 lb	0.33 kg
Toluene	0.074 lb	0.074 kg
VOC	0.40 lb	0.40 kg
Xylene	0.043 lb	0.043 kg
Solid Wastes		
Landfilled	41.6 lb	41.6 kg
Burned	3.72 lb	3.72 kg
Waste-to-Energy	1.15 lb	1.15 kg
Waterborne Wastes		
m-Xylene	8.4E-06 lb	8.4E-06 kg
1-Methylfluorene	1.4E-08 lb	1.4E-08 kg
2,4-Dimethylphenol	8.2E-06 lb	8.2E-06 kg
2-Hexanone	1.9E-06 lb	1.9E-06 kg
2-Methylnaphthalene	4.4E-06 lb	4.4E-06 kg
4-Methyl-2-Pentanone	5.1E-07 lb	5.1E-07 kg
Acetone	1.2E-06 lb	1.2E-06 kg
Acid (benzoic)	3.0E-04 lb	3.0E-04 kg
Acid (hexanoic)	6.1E-05 lb	6.1E-05 kg
Alkylated benzenes	5.5E-05 lb	5.5E-05 kg
Alkylated fluorenes	3.2E-06 lb	3.2E-06 kg
Alkylated naphthalenes	9.1E-07 lb	9.1E-07 kg
Alkylated phenanthrenes	3.8E-07 lb	3.8E-07 kg
Aluminum	0.027 lb	0.027 kg
Ammonia	0.015 lb	0.015 kg
Antimony	1.7E-05 lb	1.7E-05 kg
Arsenic	5.8E-05 lb	5.8E-05 kg
Barium	0.37 lb	0.37 kg
Benzene	3.3E-04 lb	3.3E-04 kg
Beryllium	3.6E-06 lb	3.6E-06 kg
BOD	0.42 lb	0.42 kg
Boron	9.1E-04 lb	9.1E-04 kg
Bromide	0.038 lb	0.038 kg
Cadmium	8.9E-06 lb	8.9E-06 kg
Calcium	0.62 lb	0.62 kg
Chlorides	7.64 lb	7.64 kg
Chromium (hexavalent)	1.6E-06 lb	1.6E-06 kg

Table H-1

DATA FOR THE PRODUCTION
OF HIGH-IMPACT POLYSTYRENE (HIPS) RESIN
(Cradle-to-Resin)
(page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Chromium (unspecified)	7.6E-04	lb	7.6E-04	kg
Cobalt	6.4E-06	lb	6.4E-06	kg
COD	1.07	lb	1.07	kg
Copper	7.9E-05	lb	7.9E-05	kg
Cyanide	1.0E-06	lb	1.0E-06	kg
Dibenzofuran	2.3E-08	lb	2.3E-08	kg
Dibenzothiophene	1.9E-08	lb	1.9E-08	kg
Dissolved Solids	10.5	lb	10.5	kg
Ethylbenzene	9.6E-04	lb	9.6E-04	kg
Fluorene	1.5E-06	lb	1.5E-06	kg
Iron	0.051	lb	0.051	kg
Lead	1.6E-04	lb	1.6E-04	kg
Lead 210	3.0E-14	lb	3.0E-14	kg
Lithium	0.075	lb	0.075	kg
Magnesium	0.12	lb	0.12	kg
Manganese	1.8E-04	lb	1.8E-04	kg
Mercury	3.4E-07	lb	3.4E-07	kg
Methyl Chloride	4.9E-09	lb	4.9E-09	kg
Methyl Ethyl Ketone	9.8E-09	lb	9.8E-09	kg
Molybdenum	6.7E-06	lb	6.7E-06	kg
Naphthalene	5.3E-06	lb	5.3E-06	kg
n-Decane	8.4E-06	lb	8.4E-06	kg
n-Docosane	1.3E-07	lb	1.3E-07	kg
n-Dodecane	1.6E-05	lb	1.6E-05	kg
n-Eicosane	4.4E-06	lb	4.4E-06	kg
n-Hexacosane	8.1E-08	lb	8.1E-08	kg
n-Hexadecane	1.7E-05	lb	1.7E-05	kg
Nickel	7.9E-05	lb	7.9E-05	kg
n-Octadecane	4.3E-06	lb	4.3E-06	kg
p -Xylene	3.1E-06	lb	3.1E-06	kg
o -Xylene	3.1E-06	lb	3.1E-06	kg
o-Cresol	8.4E-06	lb	8.4E-06	kg
Oil	0.031	lb	0.031	kg
Pentamethylbenzene	9.1E-09	lb	9.1E-09	kg
Phenanthrene	2.3E-07	lb	2.3E-07	kg
Phenol/ Phenolic Compounds	8.6E-04	lb	8.6E-04	kg
Phosphates	0.0010	lb	0.0010	kg
Tetradecane	6.8E-06	lb	6.8E-06	kg
Radium 226	1.1E-11	lb	1.1E-11	kg
Radium 228	5.4E-14	lb	5.4E-14	kg
Selenium	4.4E-06	lb	4.4E-06	kg
Silver	3.8E-04	lb	3.8E-04	kg
Sodium	1.81	lb	1.81	kg
Strontium	0.016	lb	0.016	kg
Styrene	9.4E-04	lb	9.4E-04	kg
Sulfates	0.013	lb	0.013	kg
Sulfides	8.7E-04	lb	8.7E-04	kg
Sulfur	7.1E-04	lb	7.1E-04	kg
Surfactants	1.5E-04	lb	1.5E-04	kg
Suspended Solids	3.14	lb	3.14	kg
Thallium	3.6E-06	lb	3.6E-06	kg
Tin	6.7E-05	lb	6.7E-05	kg
Titanium	2.6E-04	lb	2.6E-04	kg
TOC	5.9E-04	lb	5.9E-04	kg
Toluene	3.6E-04	lb	3.6E-04	kg
Total biphenyls	3.6E-06	lb	3.6E-06	kg
Total dibenzothiophenes	1.1E-08	lb	1.1E-08	kg
Vanadium	4.7E-05	lb	4.7E-05	kg
Xylene, unspecified	1.4E-04	lb	1.4E-04	kg
Yttrium	2.0E-06	lb	2.0E-06	kg
Zinc	0.061	lb	0.061	kg

References: Tables B-2 through B-5, G-2, G-3, G-4, H-2, H-3, and H-4

Source: Franklin Associates, A Division of ERG models

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

where
IO = Input/Output Matrix to produce all products/coproducts
M_{EO} = Mass of Exported Offgas
M_{Total} = Mass of all Products and Coproducts (including fuels)

No energy credit is applied for the exported fuels, since both the inputs and outputs for the exported fuels have been removed from the data set. Table H-2 shows the averaged energy and emissions data for the production of butadiene as a coproduct of olefins.

As of 2002, there were 7 butadiene producers and at least 11 butadiene plants in the U.S. (Reference H-2). While data was collected from a relatively small sample of plants, the olefins producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American butadiene production. All data collected were individually reviewed by the data providers.

To assess the quality of the data collected for butadiene, the collection method, technology, industry representation, time period, and geography were considered. The data collection methods for butadiene include direct measurements, information provided by purchasing and utility records, and estimates. The standard production technology for butadiene is the steam cracking of hydrocarbons (including natural gas liquids and petroleum liquids). The data in this module represent steam cracking of natural gas and petroleum. All data submitted for butadiene represent the year 2003 and U.S. and Canada production.

Polybutadiene Production

Polybutadiene is manufactured by solution polymerization using Ziegler-Natta catalysts. The butadiene is treated to remove inhibitors and oxygen. It is then mixed with a solvent and passed through a drying column. The purified feed is fed to the reactors containing various modifiers and catalysts. The reactor effluent is sent to blend tanks for the addition of antioxidants and is then sent to dryers. The energy requirements and environmental emissions for the production of polybutadiene are shown in Table H-3. These data are from primary and secondary sources from the 1970s and were sent to a producer for review.

Table H-2

DATA FOR THE PRODUCTION OF BUTADIENE

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs (1)							
Refined Petroleum Products	360	lb			360	kg	
Processed Natural Gas	648	lb			648	kg	
Water Consumption	216	gal			1,802	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	123	kwh		1,310	271	kwh	3.05
Electricity (cogeneration)	92.7	cu ft	(3)	104	5.79	cu meters	0.24
Natural Gas	1,212	cu ft		1,357	75.6	cu meters	3.16
Gasoline	0.0032	gal		0.45	0.027	liter	0.0011
Diesel	0.0028	gal		0.44	0.023	liter	0.0010
Internal Offgas use (2)							
From Oil	83.2	lb		2,286	83.2	kg	5.32
From Natural Gas	148	lb		4,063	148	kg	9.46
Recovered Energy	3.61	thousand Btu		3.61	8.39	MJ	0.0084
Total Process				9,117			21.2
Transportation Energy							
Combination Truck	95.0	ton-miles			306	tonne-km	
Diesel	1.00	gal		158	8.32	liter	0.37
Rail	95.0	ton-miles			306	tonne-km	
Diesel	0.24	gal		37.4	1.97	liter	0.087
Pipeline-Petroleum Products	45.0	ton-miles			145	tonne-km	
Electricity	0.98	kwh		10.0	2.16	kwh	0.023
Total Transportation				206			0.48
Environmental Emissions							
Atmospheric Emissions - Process							
Carbon Monoxide	0.0010	lb	(4)		0.0010	kg	
HCFC-022	1.0E-06	lb	(4)		1.0E-06	kg	
Hydrogen	1.0E-04	lb	(4)		1.0E-04	kg	
Hydrocarbons (NM)	0.010	lb	(4)		0.010	kg	
Methane	0.0010	lb	(4)		0.0010	kg	
Other Organics	0.0010	lb	(4)		0.0010	kg	
Particulates (unspecified)	1.0E-04	lb	(4)		1.0E-04	kg	
Particulates (PM10)	0.10	lb	(4)		0.10	kg	
Sulfur Oxides	0.0010	lb	(4)		0.0010	kg	
VOC	0.010	lb	(4)		0.010	kg	
Atmospheric Emissions - Fuel-Related (5)							
Carbon Dioxide (fossil)	997	lb			997	kg	
Carbon Monoxide	0.083	lb			0.083	kg	
Nitrogen Oxides	0.53	lb			0.53	kg	
Sulfur Oxides	0.19	lb			0.19	kg	
Solid Wastes							
Landfilled	0.042	lb			0.042	kg	
Burned	7.50	lb			7.50	kg	
Waste-to-Energy	0.0068	lb			0.0068	kg	
Waterborne Wastes							
Acetone	1.0E-08	lb	(4)		1.0E-08	kg	
Benzene	1.0E-05	lb	(4)		1.0E-05	kg	
BOD	0.010	lb	(4)		0.010	kg	
COD	0.010	lb	(4)		0.010	kg	
Ethylbenzene	1.0E-05	lb	(4)		1.0E-05	kg	
Naphthalene	1.0E-08	lb	(4)		1.0E-08	kg	
Phenol	0.0010	lb	(4)		0.0010	kg	
Styrene	1.0E-06	lb	(4)		1.0E-06	kg	
Suspended Solids	0.010	lb	(4)		0.010	kg	
Toluene	1.0E-04	lb	(4)		1.0E-04	kg	
Total Organic Carbon	0.0010	lb	(4)		0.0010	kg	
Xylene	1.0E-06	lb	(4)		1.0E-06	kg	

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(1) Specific raw 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.

(3) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(4) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(5) These fuel-related emissions were provided by the plants. These take into account the combustion of the offgas as well as the natural gas.

References: H-2 through H-5

Source: Franklin Associates, A Division of ERG

Table H-3

DATA FOR THE PRODUCTION OF POLYBUTADIENE

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Butadiene	1,015	lb		1,015	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Natural gas	2,330	cu ft	2,610	145	cu meters	6.08
Total Process			2,610			6.08
Transportation Energy						
To HIPS product						
Combination truck	450	ton-miles		1,448	tonne-km	
Diesel	4.73	gal	750	39.4	liter	1.75
Rail	30.0	ton-miles		96.5	tonne-km	
Diesel	0.074	gal	11.8	0.62	liter	0.028
Barge	440	ton-miles		1,416	ton-miles	
Diesel	0.35	gal	55.9	2.94	liter	0.13
Residual oil	1.17	gal	201	9.77	liter	0.47
Total Transportation			1,019			2.37
To ABS product						
Combination truck	223	ton-miles		718	tonne-km	
Diesel	2.34	gal	372	19.5	liter	0.87
Rail	143	ton-miles		460	tonne-km	
Diesel	0.35	gal	56.3	2.96	liter	0.13
Ocean freighter	803	ton-miles		2,584	tonne-km	
Diesel	0.15	gal	24.2	1.27	liter	0.056
Residual	1.37	gal	236	11.5	liter	0.55
Total Transportation			688			1.60
Environmental Emissions						
Atmospheric Emissions						
Hydrocarbons	13.0	lb		13.0	kg	
Solid Wastes						
Landfilled	0.10	lb		0.10	kg	
Waterborne Wastes						
BOD	0.41	lb		0.41	kg	
COD	0.83	lb		0.83	kg	
Oil	0.070	lb		0.070	kg	
Suspended Solids	1.25	lb		1.25	kg	

References: H-6 through H-9

Source: Franklin Associates, A Division of ERG

High-impact Polystyrene (HIPS) Resin

High-impact polystyrene (HIPS) resin can be produced by suspension, mass, or solution polymerization. The North American producers that provided data in this analysis use mass polymerization. HIPS is produced by the polymerization of styrene in the presence of rubber, commonly polybutadiene. The rubber is dissolved within the styrene monomer before it is sent to prepolymerization, where the stabilizers, retardants and other additives are added. Production of these stabilizers, retardants, and additives are not included in this analysis. The types and quantities of these are determined by the end-use application of the HIPS resin; this is a "generic" analysis.

Mass polymerization, also known as bulk polymerization, is one of the simplest methods of polymerization. It is often used in the polymerization of step-growth polymers. During step-growth polymerization, the functional sites of monomers react, liberate a small molecule such as water, and repeat the reaction to produce longer and longer polymer chains. Mass polymerization does not suspend the reactants in a solution such as water or organic solvents. The absence of a reaction solution makes heat control difficult and, if not monitored carefully, a mass polymerization reaction can progress too rapidly and overheating or hot spots can occur in the reaction vessel. However, since water or organic solvents are not used, there is a lower chance for contamination of the product (References H-10 and H-11).

Data for the production of HIPS resin were provided by four leading producers (6 plants) in North America. Table H-4 gives the energy requirements and emissions for the production of high-impact polystyrene resin. Scrap is produced as a coproduct during this process. A mass basis was used to partition the credit for scrap.

As of 2002 there were 12 PS producers and 24 PS plants in the U.S. (Reference H-2). These plants produce all types of polystyrene; it is unknown how many produce HIPS. While data was collected from a small sample of plants, the HIPS producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American HIPS production. The average dataset was reviewed and accepted by all HIPS data providers.

To assess the quality of the data collected for HIPS, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for HIPS include direct measurements, information provided by purchasing and utility records, and estimates. The technology represented by the HIPS data represents polymerization by mass suspension. All data submitted for HIPS ranges from 2000 through 2003 and represents U.S. production.

Table H-4

DATA FOR THE PRODUCTION OF HIGH-IMPACT POLYSTYRENE (HIPS)

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Styrene	936	lb			936	kg	
Mineral oil	18.1	lb			18.1	kg	
Polybutadiene	64.0	lb			64.0	kg	
Water Consumption	32.1	gal			268	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	51.8	kwh		533	114	kwh	1.24
Electricity (cogeneration)	44.4	cu ft	(1)	49.8	2.77	cu meter	0.12
Natural gas	354	cu ft		396	22.1	cu meter	0.92
Total Process				979			2.28
Environmental Emissions							
Atmospheric Emissions							
Acid Mist	1.0E-06	lb	(2)		1.0E-06	kg	
Carbon Monoxide	0.011	lb			0.011	kg	
HCFC-22	0.0010	lb	(2)		0.0010	kg	
Methane	0.0010	lb	(2)		0.0010	kg	
NM Hydrocarbons	0.028	lb			0.028	kg	
Nitrogen Oxides	0.038	lb			0.038	kg	
Other Organics	0.0094	lb			0.0094	kg	
Particulates (unknown)	0.016	lb			0.016	kg	
Particulates (PM10)	0.010	lb	(2)		0.010	kg	
Sulfur Oxides	1.0E-04	lb	(2)		1.0E-04	kg	
Solid Wastes							
Landfilled	3.13	lb			3.13	kg	
Burned	0.039	lb			0.039	kg	
Waste-to-Energy	1.14	lb			1.14	kg	
Waterborne Wastes							
Ammonia	1.E-04	lb	(2)		1.0E-04	kg	
BOD	1.E-04	lb	(2)		1.0E-04	kg	
Chromium	1.E-05	lb	(2)		1.0E-05	kg	
Cyanide	1.E-06	lb	(2)		1.0E-06	kg	
Dissolved solids	2.49	lb			2.49	kg	
Iron	1.E-05	lb	(2)		1.0E-05	kg	
Lead	1.E-05	lb	(2)		1.0E-05	kg	
Nickel	1.E-05	lb	(2)		1.0E-05	kg	
Oil	1.E-04	lb	(2)		1.0E-04	kg	
Phenol	1.E-06	lb	(2)		1.0E-06	kg	
Phosphates	0.0010	lb	(2)		0.0010	kg	
Suspended Solids	0.029	lb			0.029	kg	
Zinc	0.060	lb			0.060	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

References: H-6

Source: Franklin Associates, A Division of ERG

REFERENCES

H-1. APC Plastics Industry Producers' Statistics Group, as compiled by VERIS Consulting, LLC. 2004.

H-2. Chemical Profile: Butadiene. **Chemical Market Reporter.** March 18, 2002. Page 35.

H-3. Information and data collected from APC member and non-member companies producing olefins. 2004-2005.

H-4. Distances calculated using the websites: http://www.indo.com/distance/ and http://www.mapquest.com/.

H-5. Franklin Associates estimate.

H-6. Information and data collected from APC member and non-member companies producing HIPS resin. 2001-2003.

H-7. Texas Air Control Board, 1970 Emissions Data, Self-reporting System, Nonpublished data.

H-8. Texas Water Quality Board, Wastewater Effluent Report, 1972. Unpublished data extracted from Self-reporting Data. Submitted by companies located in Texas to the TWQB.

H-9. Midwest Research Institute. Private Data used for Estimates. 1974.

H-10. Kent, James A., ed. **Riegel's Handbook of Industrial Chemistry.** 10th Edition. 2003.

H-11. Radian Corporation. **Polymer Manufacturing: Technology and Health Effects.** Noyes Data Corporation, New Jersey, 1986.

APPENDIX I

POLYVINYL CHLORIDE (PVC)

INTRODUCTION

This appendix discusses the manufacture of polyvinyl chloride (PVC) resin. Over half of the PVC produced is used to manufacture pipe and siding. Almost 15 billion pounds of PVC was produced in the U.S. and Canada in 2003 (Reference I-1). The material flow for PVC resin is shown in Figure I-1. The total unit process energy and emissions data (cradle-to-PVC) for PVC are displayed in Table I-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following processes are included in this appendix:

- Salt Mining
- Sodium Hydroxide or Chlorine Production
- Hydrochloric Acid Production
- Ethylene Dichloride (EDC) Production
- Vinyl Chloride Monomer (VCM) Production
- PVC Resin

Crude oil production, distillation, desalting, and hydrotreating, natural gas production, natural gas processing, and ethylene production are discussed in Appendix B.

No fillers, additives, or plasticizers are included in this analysis; therefore, no compounding process is included.

Salt Mining

Salt (sodium chloride) is an abundant, inexpensive commodity used mostly by the chlor-alkali and other chemical industries. The various technologies used include underground mining of rock salt, solution mining of salt brine, vacuum pan salt, and solar salt. Vacuum pan salt and solar salt represent a small portion of U.S. production and are thus not included in this data module. This data module represents a mix of underground mining and solution mining techniques.

Approximately 95 percent of salt-based chlorine and caustic facilities use brine salt. In solution mining, pressurized fresh water is introduced to the bedded salt through an injection well. The brine is then pumped to the surface for treatment.

Approximately 5 percent of salt-based chlorine and caustic facilities use rock salt. Rock salt mining uses the room and pillar method. The room and pillar method excavates a series of rectangular sections, leaving columns of undisturbed salt in order to support the mine roof. After rock salt is crushed in the mine, it is transported by conveyor belts to the surface. On the surface, the rock salt is screened and prepared for shipment.

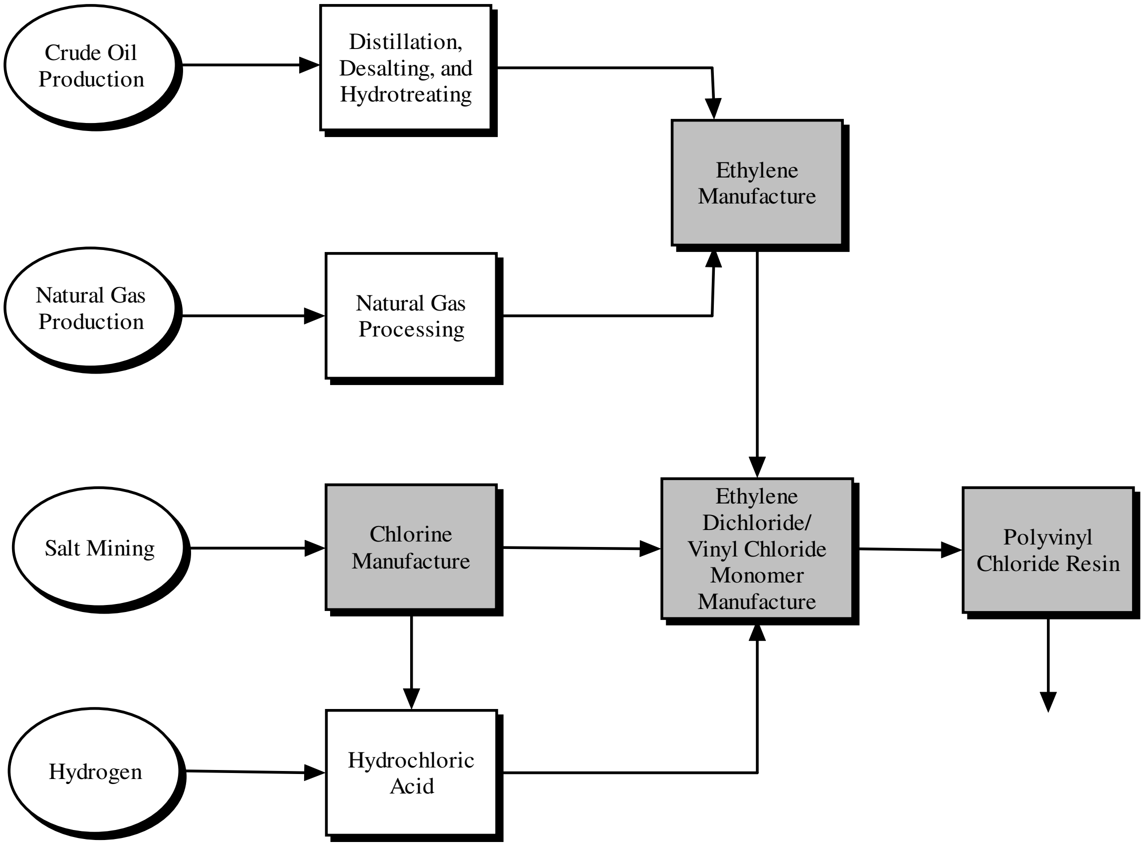

Figure I-1. Flow diagram for the manufacture of polyvinyl chloride (PVC) resin. Shaded boxes represent partial or complete data provided by manufacturers specifically for this analysis.

No data are available for the energy requirements of the solution mining of salt brine in the U.S. Energy data for the mining/extracting and purification of the salt in this analysis come from the Eco-profile of purified brine commissioned by PlasticsEurope. The transportation data was estimated from chlorine data collected from a confidential source.

Table I-1

DATA FOR THE PRODUCTION OF POLYVINYL CHLORIDE (PVC) RESIN

(Cradle-to-Resin)

(page 1 of 3)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	85.9	lb		85.9	kg	
Natural Gas	385	lb		385	kg	
Salt	552	lb		552	kg	
Oxygen	144	lb		144	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			8,248			19.2
Petroleum			1,612			3.75
Total Resource			9,860			23.0
Process Energy						
Electricity (grid)	381	kwh	4,053	840	kwh	9.44
Electricity (cogeneration)	1,690	cu ft (2)	1,893	106	cu meters	4.41
Natural gas	5,928	cu ft	6,639	370	cu meters	15.5
LPG	0.013	gal	1.46	0.11	liter	0.0034
Bit./Sbit. Coal	22.3	lb	250	22.3	kg	0.58
Distillate oil	0.75	gal	119	6.27	liter	0.28
Residual oil	0.40	gal	69.5	3.38	liter	0.16
Gasoline	0.052	gal	7.32	0.43	liter	0.017
Diesel	0.0043	gal	0.68	0.036	liter	0.0016
Internal Offgas use (1)						
From Oil	11.8	lb	363	11.8	kg	0.84
From Natural Gas	53.9	lb	1,652	53.9	kg	3.85
Recovered Energy	5.44	thousand Btu	5.44	12.7	MJ	0.013
Total Process			15,043			35.0
Transportation Energy						
Combination truck	18.7	ton-miles		60.2	tonne-km	
Diesel	0.20	gal	31.2	1.64	liter	0.073
Rail	132	ton-miles		425	tonne-km	
Diesel	0.33	gal	52.0	2.73	liter	0.12
Barge	7.81	ton-miles		25.1	tonne-km	
Diesel	0.0063	gal	0.99	0.052	liter	0.0023
Residual oil	0.021	gal	3.57	0.17	liter	0.0083
Ocean freighter	144	ton-miles		464	tonne-km	
Diesel	0.027	gal	4.35	0.23	liter	0.010
Residual	0.25	gal	42.3	2.06	liter	0.10
Pipeline-natural gas	220	ton-miles		708	tonne-km	
Natural gas	152	cu ft	170	9.47	cu meter	0.40
Pipeline-petroleum products	123	ton-miles		394	tonne-km	
Electricity	2.67	kwh	27.4	5.89	kwh	0.064
Total Transportation			332			0.77
Environmental Emissions						
Atmospheric Emissions						
Ammonia	3.4E-04	lb		3.4E-04	kg	
Antimony	2.0E-07	lb		2.0E-07	kg	
Arsenic	2.5E-08	lb		2.5E-08	kg	
Benzene	0.042	lb		0.042	kg	
Carbon Dioxide - Fossil	86.6	lb		86.6	kg	
Carbon Monoxide	0.068	lb		0.068	kg	
Carbon Tetrachloride	1.2E-04	lb		1.2E-04	kg	
CFC 13 (Methane, trichlorofluoro-)	2.1E-06	lb		2.1E-06	kg	

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table I-1

DATA FOR THE PRODUCTION
OF POLYVINYL CHLORIDE (PVC) RESIN
(Cradle-to-Resin)
(page 2 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Chlorine	0.17	lb	0.17	kg
Chromium	6.5E-08	lb	6.5E-08	kg
Dioxins (3)	1.1E-10	lb	1.1E-10	kg
Ethylbenzene	0.0050	lb	0.0050	kg
Ethylene Dibromide	4.1E-07	lb	4.1E-07	kg
HCFC-123	5.6E-05	lb	5.6E-05	kg
HCFC-22	0.0010	lb	0.0010	kg
HFC-134a	5.6E-05	lb	5.6E-05	kg
Hydrogen	0.0018	lb	0.0018	kg
Hydrogen Chloride	0.0029	lb	0.0029	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.065	lb	0.065	kg
Lead	6.8E-09	lb	6.8E-09	kg
Mercury	1.6E-05	lb	1.6E-05	kg
Methane	2.84	lb	2.84	kg
Nickel	5.5E-07	lb	5.5E-07	kg
Nitrogen Oxides	0.075	lb	0.075	kg
Non-Methane Hydrocarbons	0.042	lb	0.042	kg
Other Organics	0.046	lb	0.046	kg
Particulates (PM10)	0.062	lb	0.062	kg
Particulates (PM2.5)	0.0033	lb	0.0033	kg
Particulates (unspecified)	0.10	lb	0.10	kg
Polyaromatic Hydrocarbons (total)	5.4E-06	lb	5.4E-06	kg
Sulfur Dioxide	0.85	lb	0.85	kg
Sulfur Oxides	0.0023	lb	0.0023	kg
TOC	0.0083	lb	0.0083	kg
Toluene	0.065	lb	0.065	kg
Vinyl Chloride (4)	0.039	lb	0.039	kg
VOC	0.34	lb	0.34	kg
Xylene	0.038	lb	0.038	kg
Solid Wastes				
Landfilled	16.5	lb	16.5	kg
Burned	5.84	lb	5.84	kg
Waste-to-Energy	21.7	lb	21.7	kg
Waterborne Wastes				
m-Xylene	3.9E-06	lb	3.9E-06	kg
1-Methylfluorene	9.3E-09	lb	9.3E-09	kg
2,4-Dimethylphenol	3.7E-06	lb	3.7E-06	kg
2-Hexanone	8.7E-07	lb	8.7E-07	kg
2-Methylnaphthalene	2.1E-06	lb	2.1E-06	kg
4-Methyl-2-Pentanone	3.4E-07	lb	3.4E-07	kg
Acetone	8.2E-07	lb	8.2E-07	kg
Acid (benzoic)	1.4E-04	lb	1.4E-04	kg
Acid (hexanoic)	2.8E-05	lb	2.8E-05	kg
Alkylated benzenes	2.5E-05	lb	2.5E-05	kg
Alkylated fluorenes	1.4E-06	lb	1.4E-06	kg
Alkylated naphthalenes	4.1E-07	lb	4.1E-07	kg
Alkylated phenanthrenes	1.7E-07	lb	1.7E-07	kg
Aluminum	0.012	lb	0.012	kg
Ammonia	0.0038	lb	0.0038	kg
Antimony	7.7E-06	lb	7.7E-06	kg
Arsenic	2.5E-05	lb	2.5E-05	kg
Barium	0.17	lb	0.17	kg
Benzene	1.4E-04	lb	1.4E-04	kg
Beryllium	1.6E-06	lb	1.6E-06	kg
BOD	0.20	lb	0.20	kg
Boron	4.2E-04	lb	4.2E-04	kg
Bromide	0.016	lb	0.016	kg
Cadmium	3.9E-06	lb	3.9E-06	kg
Calcium	0.27	lb	0.27	kg
Chlorides	3.36	lb	3.36	kg
Chromium (unspecified)	4.3E-04	lb	4.3E-04	kg
Cobalt	3.0E-06	lb	3.0E-06	kg
COD	0.12	lb	0.12	kg
Copper	3.6E-05	lb	3.6E-05	kg

Table I-1

DATA FOR THE PRODUCTION
OF POLYVINYL CHLORIDE (PVC) RESIN
(Cradle-to-Resin)
(page 3 of 3)

	English units (Basis: 1,000 lb)	SI units (Basis: 1,000 kg)
Cyanide	1.0E-06 lb	1.0E-06 kg
Dibenzofuran	1.5E-08 lb	1.5E-08 kg
Dibenzothiophene	1.3E-08 lb	1.3E-08 kg
Dioxins	2.9E-10 lb	2.9E-10 kg
Dissolved Solids	30.8 lb	30.8 kg
Ethylbenzene	1.2E-05 lb	1.2E-05 kg
Fluorene	6.8E-07 lb	6.8E-07 kg
Iron	0.023 lb	0.023 kg
Lead	6.7E-05 lb	6.7E-05 kg
Lead 210	1.4E-14 lb	1.4E-14 kg
Lithium	0.066 lb	0.066 kg
Magnesium	0.054 lb	0.054 kg
Manganese	7.7E-05 lb	7.7E-05 kg
Mercury	2.6E-07 lb	2.6E-07 kg
Methyl Chloride	3.3E-09 lb	3.3E-09 kg
Methyl Ethyl Ketone	6.6E-09 lb	6.6E-09 kg
Molybdenum	3.1E-06 lb	3.1E-06 kg
Naphthalene	2.4E-06 lb	2.4E-06 kg
n-Decane	3.9E-06 lb	3.9E-06 kg
n-Docosane	8.7E-08 lb	8.7E-08 kg
n-Dodecane	7.3E-06 lb	7.3E-06 kg
n-Eicosane	2.0E-06 lb	2.0E-06 kg
n-Hexacosane	5.4E-08 lb	5.4E-08 kg
n-Hexadecane	8.0E-06 lb	8.0E-06 kg
Nickel	3.1E-05 lb	3.1E-05 kg
Nitrates	0.010 lb	0.010 kg
n-Octadecane	2.0E-06 lb	2.0E-06 kg
p -Xylene	1.4E-06 lb	1.4E-06 kg
o -Xylene	1.4E-06 lb	1.4E-06 kg
o-Cresol	3.8E-06 lb	3.8E-06 kg
Oil	0.0044 lb	0.0044 kg
p-Cresol	4.1E-06 lb	4.1E-06 kg
p-Cymene	8.1E-09 lb	8.1E-09 kg
Pentamethylbenzene	6.1E-09 lb	6.1E-09 kg
Phenanthrene	1.1E-07 lb	1.1E-07 kg
Phenol/ Phenolic Compounds	6.1E-04 lb	6.1E-04 kg
Tetradecane	3.1E-06 lb	3.1E-06 kg
Radium 226	4.8E-12 lb	4.8E-12 kg
Radium 228	2.5E-14 lb	2.5E-14 kg
Selenium	1.6E-06 lb	1.6E-06 kg
Silver	1.6E-04 lb	1.6E-04 kg
Sodium	0.77 lb	0.77 kg
Strontium	0.0073 lb	0.0073 kg
Styrene	4.5E-07 lb	4.5E-07 kg
Sulfates	0.0055 lb	0.0055 kg
Sulfides	2.2E-05 lb	2.2E-05 kg
Sulfur	3.4E-04 lb	3.4E-04 kg
Surfactants	6.6E-05 lb	6.6E-05 kg
Suspended Solids	1.56 lb	1.56 kg
Thallium	1.6E-06 lb	1.6E-06 kg
Tin	3.0E-05 lb	3.0E-05 kg
Titanium	1.2E-04 lb	1.2E-04 kg
TOC	4.5E-04 lb	4.5E-04 kg
Toluene	1.7E-04 lb	1.7E-04 kg
Total biphenyls	1.6E-06 lb	1.6E-06 kg
Total dibenzothiophenes	5.0E-09 lb	5.0E-09 kg
Vanadium	8.7E-06 lb	8.7E-06 kg
Vinyl Chloride (2)	0.0010 lb	0.0010 kg
Xylene, unspecified	6.1E-05 lb	6.1E-05 kg
Yttrium	9.0E-07 lb	9.0E-07 kg
Zinc	3.8E-04 lb	3.8E-04 kg

Note: No additives or plasticizers are included in this data.

(3) This emission was provided by the Vinyl Institute based on 2003 Dioxin TRI values and listed EDC capacity for the site assuming an operating rate at EDC capacity. Molar ratios were used to convert to units for PVC. These amounts were calculated as toxic equivalent values (TEQ).

(4) This vinyl chloride emission was provided by the Vinyl Institute, based on 2003 Vinyl Chloride TRI reported values and 2003 PVC production reported by ACC Resin Statistic Report. This value was used to represent a more industry wide average value to account for facilities that did not participate in the LCI inventory. Actual reported figures were lower than the industry average.

References: Tables B-2 through B-6 and I-2 through I-5.

Source: Franklin Associates, A Division of ERG models

No U.S. data are available for air emissions from salt mining. Since salt mining involves no chemical reactions and minimal processing requirements, it is assumed that negligible process emissions result from salt mining. Total suspended solids (TSS) are the only BPT limited water effluent from sodium chloride production (Reference I-2). No data are available for other water effluents. However, BPT limitations for sodium chloride production by solution mining stipulate that no process wastewater is returned to navigable waters. Any solution remaining after the recovery of salt brine can be returned to the body of water or salt deposit from which it originally came (Reference I-3). Salt deposits are relatively pure and require minimal beneficiation (Reference I-4). Any overburden that may be removed during rock salt mining can be returned to the mining site after the salt is recovered. Similarly, solution mining is a technology that does not generate significant amounts of solid wastes. It is thus assumed that salt mining produces negligible quantities of solid waste.

Table I-2 displays the energy requirements for the mining/extraction and purification of salt.

Sodium Hydroxide or Chlorine Production

Caustic soda (sodium hydroxide) and chlorine are produced from salt by an electrolytic process. The aqueous sodium chloride solution is electrolyzed to produce caustic soda, chlorine, and hydrogen gas.

There are three commercial processes for the electrolysis of sodium chloride: (1) the diaphragm cell process, (2) the mercury cathode cell process, and (3) the membrane cell process. Diaphragm cell electrolysis is used for 66.4 percent of production, mercury cathode cell electrolysis is used for 8.6 percent of production, and membrane cell electrolysis is used for 22.9 percent of production (Reference I-8). Membrane cell electrolysis is the most recent of these technologies and is gradually gaining commercial acceptance. Membrane cell electrolysis has relatively low energy requirements, but its high capital costs have hindered its growth (Reference I-8). Limited data are available for membrane cell electrolysis; this data module thus assigns 91.4 percent of chlorine and caustic soda production to diaphragm/membrane cell electrolysis and 8.6 percent of chlorine and caustic soda production to mercury cathode cell electrolysis (Reference I-3). The mercury cell technology is more likely to be used to produce high-purity caustic, than chlorine to be used in EDC; however, a small percentage (1.4 percent) of chlorine used in EDC does still come from mercury cells (Reference I-9).

The diaphragm cell uses graphite anodes and steel cathodes. Brine solution is passed through the anode compartment of the cell, where the salt is decomposed into chlorine gas and sodium ions. The gas is removed through a pipe at the top of the cell. The sodium ions pass through a cation-selective diaphragm. The depleted brine is either resaturated with salt or concentrated by evaporation and recycled to the cell. The sodium ions transferred across the diaphragm react with water at the cathode to produce hydrogen and sodium hydroxide. Diffusion of the cathode products back into the brine solution is prevented by the diaphragm.

The mercury cell uses graphite anodes and mercury cathodes. Sodium reacts with the mercury cathode to produce an amalgam (an alloy of mercury and sodium) that is sent to another compartment of the cell and reacted with water to produce hydrogen and high purity sodium hydroxide. The chemistry that occurs at the mercury cathode includes the following reactions:

$NaCl + xHg \rightarrow 1/2\ Cl_2 + Na(Hg)x$ and
$Na(Hg)x + H_2O \rightarrow NaOH + 1/2H_2 + xHg$

Mercury loss is a disadvantage of the mercury cathode cell process. Some of the routes by which mercury can escape are in the hydrogen gas stream, in cell room ventilation air and washing water, through purging of the brine loop and disposal of brine sludges, and through end box fumes.

Table I-2

DATA FOR THE MINING OF SALT

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	15.1	kwh	155	33.3	kwh	0.36
Natural gas	397	cu ft	445	24.8	cu meters	1.04
Bit./Sbit. Coal	11.7	lb	131	11.7	kg	0.31
Distillate oil	1.21	gal	192	10.1	liter	0.45
Total Process			924			2.15
Transportation Energy						
Rail	1.25	ton-miles		4.02	tonne-km	
Diesel	0.0031	gal	0.49	0.026	liter	0.0011
Barge	1.25	ton-miles		4.02	tonne-km	
Diesel	0.0010	gal	0.16	0.0083	liter	3.7E-04
Residual oil	0.0033	gal	0.57	0.028	liter	0.0013
Pipeline-petroleum products	114	ton-miles		367	tonne-km	
Electricity	2.49	kwh	25.5	5.48	kwh	0.059
Total Transportation			26.7			0.062

References: I-5 through I-7

Source: Franklin Associates, A Division of ERG

Titanium anodes, coated with metal oxide finishes, are gaining commercial acceptance and are gradually replacing graphite anodes. The advantages of titanium anodes are (1) corrosion resistance and (2) the low activation energy for electrolysis at the anode surface (Reference I-10).

The reason coproduct credit was given is that it is not possible, using the electrolytic cell, to get chlorine from salt without also producing sodium hydroxide and hydrogen, both of which have commercial value as useful coproducts. Likewise, sodium hydroxide cannot be obtained without producing the valuable coproducts of chlorine and hydrogen. Furthermore, it is not possible to control the cell to increase or decrease the amount of chlorine or caustic soda resulting from a given input of salt. This is determined by the stoichiometry of the reaction; the electrolysis of sodium chloride produces approximately 1.1 tons caustic soda per ton of chlorine. Caustic soda is usually handled and sold as a 50% solution in water.

The energy requirements and environmental emissions for the production of sodium hydroxide or chlorine are given in Tables I-3a and I-3b. Diaphragm and mercury cells are considered as the main source of chlorine/caustic in this analysis. Data was collected from one plant that used both the diaphragm and membrane technologies, and so their dataset represented both cells. According to a study performed by Chemical Market Associates, Inc. (CMAI), the approximate amount of chlorine from mercury cell technology going into U.S. EDC production is 1.4 percent. Two percent of the chlorine used by EDC plants is assumed to come from the mercury cell technology as shown in Table I-3a. For the overall chlorine/caustic industry, it is estimated that 91.4 percent of the cell technology is diaphragm and membrane, while 8.6 percent of the cell technology is mercury. The collected datasets were weighted using these fractions in Table I-3b.

As of 2003 there were 20 chlorine/caustic producers and 41 chlorine/caustic plants in the U.S. for the three standard technologies (Reference I-7). The chlorine/caustic data collected for this module represent 1 producer and 3 plants in the U.S. Besides this recently collected data, 2 diaphragm cell datasets and 2 mercury cell datasets were used from the early 1990s. While data was collected from a small sample of plants, the chlorine/caustic producer who provided data for this module verified that the characteristics of their plant are representative of the diaphragm/membrane cell technology for North American chlorine/caustic production. The average dataset was reviewed and accepted by the chlorine/caustic data provider.

One of the five company datasets was collected for this project and represents 2003 data, while the other four datasets comes from 1989-1992. The 2003 data were collected from direct measurements, calculated from equipment specifications, taken from purchasing/utility records, and engineering estimates. The collection methods for the older data are unknown.

Hydrochloric Acid Production

Although there are a number of processes used to produce hydrochloric acid, this analysis assumes that it is produced from the synthesis of the elements hydrogen and chloride ($H_2 + Cl_2 \rightarrow 2HCl$). Most hydrochloric acid used in the production of EDC comes from producing VCM. However, some EDC producers must supplement the amount of hydrochloric acid.

The dataset used in this analysis for hydrochloric acid comes from the ecoinvent Database. It is shown in Table I-4 as a cradle-to-gate process due to confidentiality issues concerning showing unit process data from the EcoInvent Database. The dataset itself is provided by Swiss Centre for LCI, EMPA from the 2007 Life Cycle Inventories of Chemicals. The dataset states that the data represents a cross-section of actual plants in Europe for the years 1997-2000.

Ethylene Dichloride (EDC) Production

Ethylene dichloride is produced from the reaction of ethylene and chlorine. Ethylene is chlorinated in the liquid phase at a temperature of 20° to 120° C and a pressure of 75 psi. A ferric chloride catalyst is used to drive the reaction. The crude product from the reactor is then purified by distillation to yield ethylene dichloride. Ethylene dichloride data was collected with VCM data and are included within the VCM dataset (Table I-5).

Vinyl Chloride Monomer (VCM) Production

Vinyl chloride monomer (VCM) is produced almost exclusively by thermal cleavage (dehydrochlorination) of ethylene dichloride. The ethylene dichloride is fed to the cracking unit to form VCM and HCl. The HCl from this process is fed back to the ethylene dichloride reaction. In the case of the collected EDC/VCM data, either the producer used all HCl produced or not enough HCl was produced, and supplemental HCl was purchased. Unreacted ethylene dichloride is separated from the VCM.

Data for the production of EDC/VCM were provided by three leading producers (3 plants) in North America to Franklin Associates under contract to Plastics Division of the American Chemistry Council (ACC). The energy requirements and environmental emissions for the production of EDC/VCM are shown in Table I-5. Dichloroethane is produced as a coproduct during this process. A mass basis was used to partition the credit for this coproduct.

Table I-3a

DATA FOR THE PRODUCTION OF SODIUM HYDROXIDE OR CHLORINE (98.6% Diaphragm/Membrane and 1.4% Mercury Technologies)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Salt	892	lb		892	kg	
Water Consumption	384	gal		3,204	liter	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	277	kwh	2,851	611	kwh	6.64
Electricity (cogeneration)	1,126	cu ft (1)	1,261	70.3	cu meters	2.93
Natural gas	1,945	cu ft	2,178	121	cu meters	5.07
Bit./Sbit. Coal	25.6	lb	287	25.6	kg	0.67
Residual oil	0.060	gal	10.3	0.50	liter	0.024
Total Process			6,587			15.3
Transportation Energy						
Combination truck	24.6	ton-miles		79.2	tonne-km	
Diesel	0.26	gal	41.0	2.16	liter	0.10
Rail	66.5	ton-miles		214	tonne-km	
Diesel	0.16	gal	26.2	1.38	liter	0.061
Pipeline-petroleum products	2.60	ton-miles		8.37	tonne-km	
Electricity	0.057	kwh	0.58	0.12	kwh	0.0014
Total Transportation			67.8			0.16
Environmental Emissions						
Atmospheric Emissions						
Benzene	2.2E-05	lb		2.2E-05	kg	
Carbon Dioxide (fossil)	0.074	lb		0.074	kg	
Carbon Monoxide	1.4E-04	lb		1.4E-04	kg	
Carbon Tetrachloride	1.9E-04	lb		1.9E-04	kg	
Chlorine	0.0011	lb		0.0011	kg	
HFCs/HCFCs	1.8E-04	lb		1.8E-04	kg	
NM Hydrocarbons	2.7E-04	lb		2.7E-04	kg	
Hydrogen Chloride	3.2E-04	lb		3.2E-04	kg	
Lead	1.1E-08	lb		1.1E-08	kg	
Mercury	2.6E-05	lb		2.6E-05	kg	
Methane	1.1E-06	lb		1.1E-06	kg	
Nitrogen Oxides	0.0038	lb		0.0038	kg	
Other Organics	8.0E-06	lb		8.0E-06	kg	
Particulates	0.0028	lb		0.0028	kg	
PM2.5	1.2E-04	lb		1.2E-04	kg	
PM10	0.021	lb		0.021	kg	
Sulfur Oxides	5.5E-04	lb		5.5E-04	kg	
Solid Wastes						
Landfilled	0.63	lb		0.63	kg	
Burned	1.42	lb		1.42	kg	
Waterborne Wastes						
BOD	0.27	lb		0.27	kg	
Copper	1.2E-07	lb		1.2E-07	kg	
Dissolved Solids	44.3	lb		44.3	kg	
Lead	5.6E-07	lb		5.6E-07	kg	
Mercury	2.0E-07	lb		2.0E-07	kg	
Nickel	5.8E-07	lb		5.8E-07	kg	
Sulfides	7.3E-06	lb		7.3E-06	kg	
Suspended Solids	0.080	lb		0.080	kg	
Zinc	5.6E-07	lb		5.6E-07	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

Note: According to a study performed by Chemical Market Associates, Inc. (CMAI), the approximate amount of chlorine from mercury cell technology going into EDC production is 1.4 percent. This dataset assumes 98.6 percent of the chlorine used by EDC plants comes from the diaphragm/membrane technology.

References: I-6, I-11, I-12, and I-14

Source: Franklin Associates, A Division of ERG

Table I-3b

**DATA FOR THE PRODUCTION
OF SODIUM HYDROXIDE OR CHLORINE
(91.4% Diaphragm/Membrane and 8.6% Mercury Technologies)**

	English units (Basis: 1,000 lb)		Total Energy Thousand Btu	SI units (Basis: 1,000 kg)		Total Energy GigaJoules
Material Inputs						
Salt	884	lb		884	kg	
Water Consumption	384	gal		3,204	liter	
Energy Usage						
Process Energy						
Electricity (grid)	306	kwh	3,149	675	kwh	7.33
Electricity (cogeneration)	1039	cu ft (1)	1,164	64.9	cu meters	2.71
Natural gas	1,821	cu ft	2,040	114	cu meters	4.75
Bit./Sbit. Coal	25.0	lb	281	25.0	kg	0.65
Residual oil	0.15	gal	25.7	1.25	liter	0.060
Total Process			6,659			15.5
Transportation Energy						
Used in Rigid and Flexible Polyols						
Combination truck	67.4	ton-miles		217	tonne-km	
Diesel	0.71	gal	112	5.91	liter	0.26
Rail	20.6	ton-miles		66.3	tonne-km	
Diesel	0.05	gal	8.11	0.43	liter	0.019
Total Transportation			120			0.28
Used in MDI and TDI						
Pipeline-petroleum products	1.25	ton-miles		4.01	tonne-km	
Electricity	0.027	kwh	0.28	0.060	kwh	6.5E-04
Total Transportation			0.28			6.5E-04
Environmental Emissions						
Atmospheric Emissions						
Benzene	2.1E-05	lb		2.1E-05	kg	
Carbon Dioxide (fossil)	0.069	lb		0.069	kg	
Carbon Monoxide	1.3E-04	lb		1.3E-04	kg	
Carbon Tetrachloride	1.8E-04	lb		1.8E-04	kg	
Chlorine	0.0011	lb		0.0011	kg	
HCFC-123	8.5E-05	lb		8.5E-05	kg	
HFC-134a	8.5E-05	lb		8.5E-05	kg	
NM Hydrocarbons	2.5E-04	lb		2.5E-04	kg	
Hydrogen Chloride	3.0E-04	lb		3.0E-04	kg	
Lead	1.0E-08	lb		1.0E-08	kg	
Mercury	1.6E-04	lb		1.6E-04	kg	
Methane	9.9E-07	lb		9.9E-07	kg	
Nitrogen Oxides	0.0035	lb		0.0035	kg	
Other Organics	7.4E-06	lb		7.4E-06	kg	
Particulates	0.0027	lb		0.0027	kg	
PM2.5	1.1E-04	lb		1.1E-04	kg	
PM10	0.019	lb		0.019	kg	
Sulfur Oxides	5.1E-04	lb		5.1E-04	kg	
Solid Wastes						
Landfilled	1.20	lb		1.20	kg	
Burned	1.32	lb		1.32	kg	
Waterborne Wastes						
BOD	0.25	lb		0.25	kg	
Copper	1.1E-07	lb		1.1E-07	kg	
Dissolved Solids	41.0	lb		41.0	kg	
Lead	5.2E-07	lb		5.2E-07	kg	
Mercury	5.1E-07	lb		5.1E-07	kg	
Nickel	5.4E-07	lb		5.4E-07	kg	
Sulfides	4.5E-05	lb		4.5E-05	kg	
Suspended Solids	0.074	lb		0.074	kg	
Zinc	5.2E-07	lb		5.2E-07	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

References: I-6, I-11, I-12, and I-14

Source: Franklin Associates, A Division of ERG

Table I-4

DATA FOR THE PRODUCTION OF HYDROCHLORIC ACID

(Cradle-to-Gate)

(Page 1 of 3)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			1,878			4.37
Process Energy						
Electricity (grid)	439	kwh	4,517	968	kwh	10.5
Electricity (cogeneration)	1,097	cu ft (1)	1,229	68.5	cu meters	2.86
Natural gas	2,358	cu ft	2,641	147	cu meters	6.15
Coal (bituminous)	35.1	lb	395	35.1	kg	0.92
Distillate oil	1.06	gal	169	8.89	liter	0.39
Residual oil	0.067	gal	11.4	0.56	liter	0.027
Gasoline	0.0071	gal	1.00	0.059	liter	0.0023
Total Process			8,963			20.9
Transportation Energy						
Combination truck	24.4	ton-miles		78.4	tonne-km	
Diesel	0.26	gal	40.6	2.14	liter	0.095
Rail	66.3	ton-miles		213	tonne-km	
Diesel	0.16	gal	26.1	1.37	liter	0.061
Barge	1.09	ton-miles		3.50	tonne-km	
Diesel	8.7E-04	gal	0.14	0.0073	liter	3.2E-04
Residual oil	0.0029	gal	0.50	0.024	liter	0.0012
Pipeline-natural gas	39.3	ton-miles		126	tonne-km	
Natural gas	27.1	cu ft	30.3	1.69	cu meter	0.071
Pipeline-petroleum products	104	ton-miles		334	tonne-km	
Electricity	2.26	kwh	23.2	4.98	kwh	0.054
Total Transportation			121			0.28
Environmental Emissions (Process)						
Atmospheric Emissions						
Benzene	0.0076	lb		0.0076	kg	
Carbon Dioxide (Fossil)	222	lb		222	kg	
Carbon Monoxide	0.19	lb		0.19	kg	
Carbon Tetrachloride	1.9E-04	lb		1.9E-04	kg	
Chlorine	1.90	lb		1.90	kg	
Ethylbenzene	9.4E-04	lb		9.4E-04	kg	
HCFC-123	8.8E-05	lb		8.8E-05	kg	
HFC-134a	8.8E-05	lb		8.8E-05	kg	
Hydrogen Chloride	3.1E-04	lb		3.1E-04	kg	
Lead	1.1E-08	lb		1.1E-08	kg	
Mercury	2.5E-05	lb		2.5E-05	kg	
Methane	1.11	lb		1.11	kg	
Nitrogen Oxides	0.0037	lb		0.0037	kg	
Non-Methane Hydrocarbons	2.6E-04	lb		2.6E-04	kg	
Other Organics	7.8E-06	lb		7.8E-06	kg	
Particulates (PM10)	0.020	lb		0.020	kg	
Particulates (PM2.5)	1.2E-04	lb		1.2E-04	kg	
Particulates (unspecified)	0.0027	lb		0.0027	kg	

(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

Table I-4

DATA FOR THE PRODUCTION OF HYDROCHLORIC ACID

(Cradle-to-Gate)

(Page 2 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Sulfur Oxides	1.91	lb	1.91	kg
TOC	0.097	lb	0.097	kg
Toluene	0.012	lb	0.012	kg
VOC	0.060	lb	0.060	kg
Xylene	0.0068	lb	0.0068	kg
Solid Wastes				
Landfilled	2.61	lb	2.61	kg
Burned	1.38	lb	1.38	kg
Waterborne Wastes				
1-Methylfluorene	3.9E-08	lb	3.9E-08	kg
2,4-Dimethylphenol	9.7E-06	lb	9.7E-06	kg
2-Hexanone	2.3E-06	lb	2.3E-06	kg
2-Methylnaphthalene	5.5E-06	lb	5.5E-06	kg
4-Methyl-2-Pentanone	1.5E-06	lb	1.5E-06	kg
Acetone	3.5E-06	lb	3.5E-06	kg
Acid (benzoic)	3.5E-04	lb	3.5E-04	kg
Acid (hexanoic)	7.3E-05	lb	7.3E-05	kg
Alkalinity	0.028	lb	0.028	kg
Alkylated benzenes	3.4E-06	lb	3.4E-06	kg
Alkylated fluorenes	2.0E-07	lb	2.0E-07	kg
Alkylated naphthalenes	5.6E-08	lb	5.6E-08	kg
Alkylated phenanthrenes	2.3E-08	lb	2.3E-08	kg
Aluminum	0.0064	lb	0.0064	kg
Ammonia	0.0043	lb	0.0043	kg
Antimony	3.9E-06	lb	3.9E-06	kg
Arsenic	7.7E-05	lb	7.7E-05	kg
Barium	0.099	lb	0.099	kg
Benzene	5.8E-04	lb	5.8E-04	kg
Beryllium	3.5E-06	lb	3.5E-06	kg
BOD	0.32	lb	0.32	kg
Boron	0.0011	lb	0.0011	kg
Bromide	0.074	lb	0.074	kg
Cadmium	1.1E-05	lb	1.1E-05	kg
Calcium	1.12	lb	1.12	kg
Chlorides	12.5	lb	12.5	kg
Chromium (unspecified)	1.8E-04	lb	1.8E-04	kg
Cobalt	7.7E-06	lb	7.7E-06	kg
COD	0.10	lb	0.10	kg
Copper	4.9E-05	lb	4.9E-05	kg
Cyanide	2.5E-08	lb	2.5E-08	kg
Dibenzofuran	6.6E-08	lb	6.6E-08	kg
Dibenzothiophene	5.3E-08	lb	5.3E-08	kg
Dissolved Solids	58.7	lb	58.7	kg
Ethylbenzene	3.3E-05	lb	3.3E-05	kg
Fluorine	1.2E-07	lb	1.2E-07	kg
Hardness	3.44	lb	3.44	kg
Iron	0.020	lb	0.020	kg
Lead	1.1E-04	lb	1.1E-04	kg
Lead 210	3.6E-14	lb	3.6E-14	kg

Table I-4

DATA FOR THE PRODUCTION OF HYDROCHLORIC ACID

(Cradle-to-Gate)

(Page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Lithium	0.37	lb	0.37	kg
Magnesium	0.22	lb	0.22	kg
Manganese	3.5E-04	lb	3.5E-04	kg
Mercury	2.6E-07	lb	2.6E-07	kg
Methyl Chloride	1.4E-08	lb	1.4E-08	kg
Methyl Ethyl Ketone	2.8E-08	lb	2.8E-08	kg
Molybdenum	8.0E-06	lb	8.0E-06	kg
m-Xylene	1.1E-05	lb	1.1E-05	kg
Naphthalene	6.3E-06	lb	6.3E-06	kg
n-Decane	1.0E-05	lb	1.0E-05	kg
n-Docosane	3.7E-07	lb	3.7E-07	kg
n-Dodecane	1.9E-05	lb	1.9E-05	kg
n-Eicosane	5.3E-06	lb	5.3E-06	kg
n-Hexacosane	2.3E-07	lb	2.3E-07	kg
n-Hexadecane	2.1E-05	lb	2.1E-05	kg
n-Octadecane	5.2E-06	lb	5.2E-06	kg
n-Tetradecane	8.4E-06	lb	8.4E-06	kg
Nickel	6.1E-05	lb	6.1E-05	kg
o + p-Xylene	7.7E-06	lb	7.7E-06	kg
o-Cresol	1.0E-05	lb	1.0E-05	kg
Oil	0.0067	lb	0.0067	kg
p-Cresol	1.1E-05	lb	1.1E-05	kg
p-Cymene	3.5E-08	lb	3.5E-08	kg
Pentamethylbenzene	2.6E-08	lb	2.6E-08	kg
Phenanthrene	4.4E-08	lb	4.4E-08	kg
Phenol/Phenolic Compounds	1.6E-04	lb	1.6E-04	kg
Radium 226	1.3E-11	lb	1.3E-11	kg
Radium 228	6.4E-14	lb	6.4E-14	kg
Selenium	7.7E-07	lb	7.7E-07	kg
Silver	7.3E-04	lb	7.3E-04	kg
Sodium	3.54	lb	3.54	kg
Strontium	0.019	lb	0.019	kg
Sulfates	0.026	lb	0.026	kg
Sulfides	7.1E-06	lb	7.1E-06	kg
Sulfur	9.2E-04	lb	9.2E-04	kg
Surfactants	3.5E-04	lb	3.5E-04	kg
Suspended Solids	0.30	lb	0.30	kg
Thallium	8.2E-07	lb	8.2E-07	kg
Tin	3.8E-05	lb	3.8E-05	kg
Titanium	6.0E-05	lb	6.0E-05	kg
Toluene	5.5E-04	lb	5.5E-04	kg
Total biphenyls	2.2E-07	lb	2.2E-07	kg
Total dibenzothiophenes	6.8E-10	lb	6.8E-10	kg
Vanadium	9.4E-06	lb	9.4E-06	kg
Xylene (unspecified)	2.8E-04	lb	2.8E-04	kg
Yttrium	2.3E-06	lb	2.3E-06	kg
Zinc	1.7E-04	lb	1.7E-04	kg

Reference: I-16

Source: Franklin Associates, A Division of ERG

Table I-5

DATA FOR THE PRODUCTION OF
ETHYLENE DICHLORIDE (EDC)/VINYL CHLORIDE MONOMER (VCM)

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Ethylene	453	lb			453	kg	
Chlorine	535	lb			535	kg	
Oxygen	144	lb			144	kg	
Hydrochloric acid	85.4	lb			85.4	kg	
Water Consumption	104	gal			868	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	68.6	kwh		706	151	kwh	1.64
Electricity (cogeneration)	628	cu ft	(1)	704	39.2	cu meters	1.64
Natural gas	2,006	cu ft		2,247	125	cu meters	5.23
Total Process				3,656			8.51
Transportation Energy							
Rail	87.2	ton-miles			280	tonne-km	
Diesel	0.22	gal		34.3	1.80	liter	0.080
Pipeline-petroleum products	1.20	ton-miles			3.86	tonne-km	
Electricity	0.026	kwh		0.27	0.058	kwh	6.2E-04
Total Transportation				34.6			0.080
Environmental Emissions							
Atmospheric Emissions							
Carbon Monoxide	0.011	lb			0.011	kg	
Carbon Dioxide	37.3	lb			37.3	kg	
Chlorine	0.0010	lb	(2)		0.0010	kg	
Hydrochloric Acid	0.0026	lb			0.0026	kg	
Nitrogen Oxides	0.032	lb			0.032	kg	
Other Organics	0.0069	lb	(3)		0.0069	kg	
Particulates (unknown)	0.010	lb	(2)		0.010	kg	
PM2.5	0.0010	lb	(2)		0.0010	kg	
PM10	0.0010	lb	(2)		0.0010	kg	
Solid Wastes							
Landfilled	0.36	lb			0.36	kg	
Burned	3.32	lb			3.32	kg	
Waste-to-Energy	21.7	lb			21.7	kg	
Waterborne Wastes							
Chlorides	1.0E-05	lb	(2)		1.0E-05	kg	
Copper	1.0E-07	lb	(2)		1.0E-07	kg	
Vinyl Chloride	0.0010	lb	(4)		0.0010	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(3) This category contains small amounts of EDC and VCM as well as other hydrocarbons which were not separated out by the data providers. These amounts may be overcounting the VCM emissions as the Vinyl Institute provided atmospheric VCM emissions for the production of EDC/VCM/PVC as shown in Table I-5.

(4) This vinyl chloride emission was provided by the Vinyl Institute, based on 2003 Vinyl Chloride TRI reported values and 2003 PVC production reported by ACC Resin Statistic Report. This value was used to represent a more industry wide average value to account for facilities that did not participate in the LCI inventory. Actual reported figures were lower than the industry average.

References: I-6, I-14, and I-15.

Source: Franklin Associates, A Division of ERG

As of 2003 there were 8 VCM producers and 12 VCM plants in the U.S. (Reference I-13). While data was collected from a small sample of plants, the EDC/VCM producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American EDC/VCM production. The average dataset was reviewed and accepted by all EDC/VCM data providers.

To assess the quality of the data collected for EDC/VCM, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for EDC/VCM include direct measurements, information provided by purchasing and utility records, calculated from equipment specifications, and engineering estimates. All data submitted for EDC/VCM ranges from 2003-2004 and represents U.S. production.

PVC Resin Production

PVC resin is produced by suspension, emulsion, mass, or solution polymerization of VCM. The data presented in this appendix represents suspension polymerization.

In the suspension process, VCM and initiators are mixed with water and kept in the form of aqueous droplets by agitation and suspension stabilizers. The polymerization generally is carried out in a nitrogen atmosphere in large agitated reactors. The reaction time is typically about 12 hours, and conversion of VCM approaches 90 percent. After polymerization, the unreacted monomer is removed and recycled. The polymer is blended with additives and modifiers and centrifuged to remove water. The resin is then dried and packaged for shipment.

Table I-6 presents the data for the production of PVC resin by suspension polymerization. Data for the production of PVC were provided by three leading producers (3 plants) in North America to Franklin Associates under contract to Plastics Division of the American Chemistry Council (ACC). Scrap is produced as a coproduct during this process. A mass basis was used to partition the credit for the scrap.

As of 2003 there were 12 PVC producers and 25 PVC plants in the U.S. (Reference I-7). While data was collected from a small sample of plants, the PVC producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American PVC suspension technology production. The average dataset was reviewed and accepted by all PVC data providers.

To assess the quality of the data collected for PVC, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for PVC include direct measurements, information provided by purchasing and utility records, calculated from equipment specifications, and engineering estimates. All data submitted for PVC ranges from 2003-2004 and represents U.S. production.

Table I-6

DATA FOR THE PRODUCTION OF POLYVINYL CHLORIDE (PVC) RESIN

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Vinyl Chloride Monomer	1,001	lb			1,001	kg	
Water Consumption	121	gal			1,010	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	74.4	kwh		766	164	kwh	1.78
Electricity (cogeneration)	273	cu ft	(1)	306	17.1	cu meters	0.71
Natural gas	925	cu ft		1,036	57.7	cu meters	2.41
Total Process				2,108			4.91
Environmental Emissions							
Atmospheric Emissions							
Chlorine	0.010	lb	(2)		0.010	kg	
HCFC-22	0.0010	lb	(2)		0.0010	kg	
Hydrochloric Acid	1.0E-04	lb	(2)		1.0E-04	kg	
Other Organics	0.039	lb			0.039	kg	
Particulates (unknown)	0.087	lb			0.087	kg	
Vinyl Chloride	0.039	lb	(3)		0.039	kg	
Dioxins	1.1E-10	lb	(4)		1.1E-10	kg	
Solid Wastes							
Landfilled	1.09	lb			1.09	kg	
Burned	5.2E-04	lb			5.2E-04	kg	
Waterborne Wastes							
Ammonia	0.0010	lb	(2)		0.0010	kg	
BOD	0.012	lb			0.012	kg	
Chromium (unknown)	1.0E-04	lb	(2)		1.0E-04	kg	
COD	0.068	lb			0.068	kg	
Cyanide	1.0E-06	lb	(2)		1.0E-06	kg	
Nitrates	0.010	lb	(2)		0.010	kg	
Oil	0.0010	lb	(2)		0.0010	kg	
Phenol	9.9E-05	lb			9.9E-05	kg	
Suspended solids	0.16	lb			0.16	kg	
Zinc	1.0E-04	lb	(2)		1.0E-04	kg	
Dioxins	2.9E-10	lb	(4)		2.9E-10	kg	

Note: No additives or plasticizers were included in this data.

(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(3) This vinyl chloride emission was provided by the Vinyl Institute, based on 2003 Vinyl Chloride TRI reported values and 2003 PVC production reported by ACC Resin Statistic Report. This amount includes both the EDC/VCM plant as well as the PVC plant. This value was used to represent a more industry wide average value to account for facilities that did not participate in the LCI inventory. Actual reported figures were lower than the industry average.

(4) This emission was provided by the Vinyl Institute based on 2003 Dioxin TRI values and listed EDC capacity for the site assuming an operating rate at EDC capacity. Molar ratios were used to convert to units for PVC. These amounts were calculated as toxic equivalent values (TEQ).

References: I-15

Source: Franklin Associates, A Division of ERG

REFERENCES

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APPENDIX J

ACRYLONITRILE-BUTADIENE-STYRENE (ABS)

INTRODUCTION

This appendix discusses the manufacture of acrylonitrile-butadiene-styrene (ABS) resin. ABS is used to manufacture boats, mobile homes, luggage, and pipelines. Approximately 1.37 billion pounds of ABS were produced in the U.S., Mexico, and Canada in 2004 (Reference J-1). The material flow for ABS resin is shown in Figure J-1. The total unit process energy and emissions data (cradle-to-ABS) for ABS are displayed in Table J-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following processes are included in this appendix:

- Ammonia Production
- Acrylonitrile Production
- ABS Resin

Crude oil production, distillation, desalting, and hydrotreating, natural gas production, natural gas processing, and ethylene production are discussed in Appendix B. Propylene production is discussed in Appendix E. Pygas production, benzene production, and ethylbenzene/styrene production are discussed in Appendix G. Butadiene production and polybutadiene production are discussed in Appendix H.

Ammonia Production

Ammonia is produced primarily by steam reforming natural gas. Natural gas is fed with steam into a tubular furnace where the reaction over a nickel reforming catalyst produces hydrogen and carbon oxides. The primary reformer products are then mixed with preheated air and reacted in a secondary reformer to produce the nitrogen needed in ammonia synthesis. The gas is then cooled to a lower temperature and subjected to the water shift reaction in which carbon monoxide and steam are reacted to form carbon dioxide and hydrogen. The carbon dioxide is removed from the shifted gas in an absorbent solution. Hydrogen and nitrogen are reacted in a synthesis converter to form ammonia (Reference J-2).

Table J-2 presents the energy and emissions data for the production of ammonia. The energy data for ammonia was calculated from secondary sources (Reference J-2) and from stoichiometry. The transportation data was estimated from the ammonia and acrylonitrile chemical profiles (Reference J-3) and from the acrylonitrile data provider. The atmospheric emissions and solid wastes are estimates, while the waterborne emissions are from a 1970's source (Reference J-4), although these emissions were reviewed and revised in 1994.

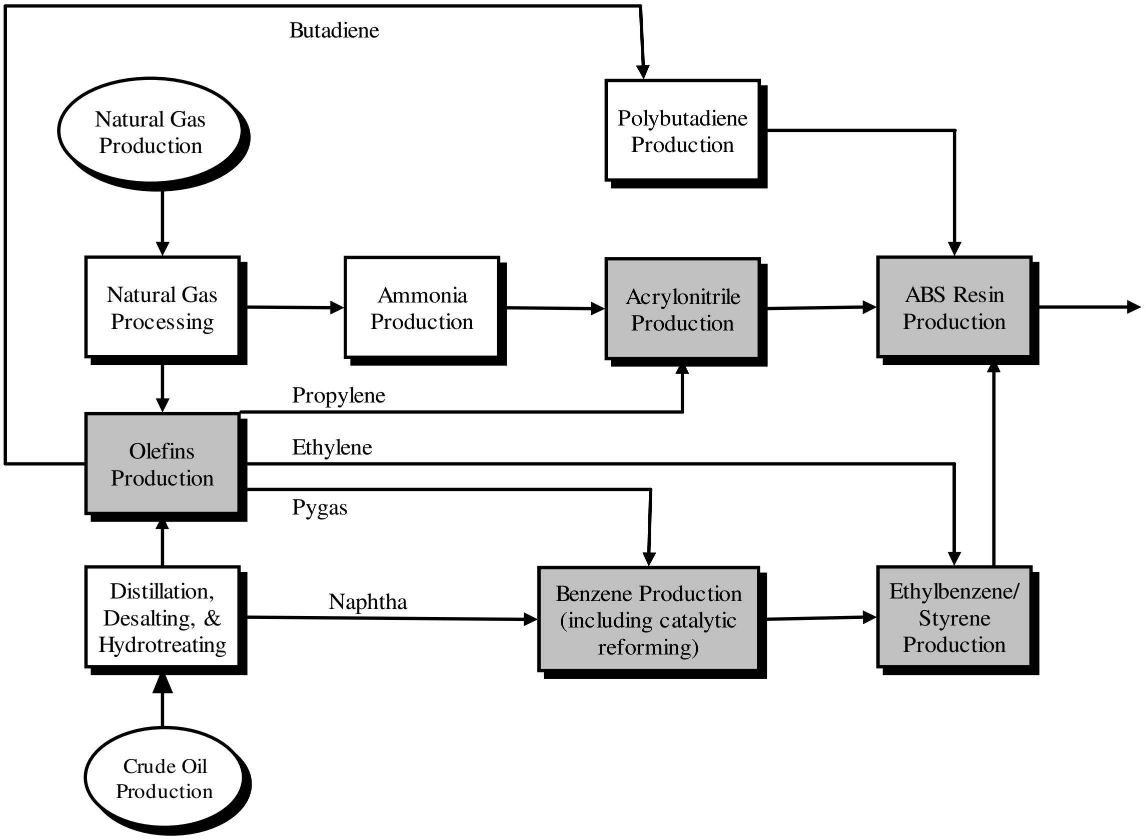

Figure J-1. Flow diagram for the production of acrylonitrile-butadiene-styrene (ABS) resin. Shaded boxes represent partial or complete data provided by manufacturers specifically for this analysis.

Acrylonitrile Production

Acrylonitrile production in the U.S. and most of the world is based on the Sohio process. Propylene, air, and ammonia are catalytically converted to acrylonitrile using a fluidized bed reactor. Operating temperatures are 400° to 500° Celsius and gauge pressures are 30 to 300 kPa. The reaction is exothermic with recovered heat being used to generate steam for use in the process. The chemical equation for the process is:

$$2CH_2{=}CH\text{-}CH_3 + 2NH_3 + 3O_2 \rightarrow 2CH_2{=}CH\text{-}CN + 6H_2O$$

Major by-products are hydrogen cyanide and acetonitrile, which are normally incinerated because supply often exceeds demand. Unused ammonia can be recovered as ammonium sulfate and then disposed of, but it is commonly vented to the atmosphere (Reference J-2).

Table J-1

DATA FOR THE PRODUCTION
OF ACRYLONITRILE-BUTADIENE-STYRENE (ABS) RESIN
(Cradle-to-Resin)
(page 1 of 3)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	602	lb		602	kg	
Natural Gas	529	lb		529	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			11,320			26.4
Petroleum			11,291			26.3
Total Resource			22,610			52.6
Process Energy						
Electricity (grid)	504	kwh	5,366	1,112	kwh	12.5
Electricity (cogeneration)	246	cu ft (2)	275	15.3	cu meters	0.64
Natural gas	8,778	cu ft	9,832	548	cu meters	22.9
LPG	0.090	gal	9.75	0.75	liter	0.023
Bit./Sbit. Coal	68.4	lb	768	68.4	kg	1.79
Distillate oil	0.41	gal	64.6	3.40	liter	0.15
Residual oil	4.31	gal	739	35.9	liter	1.72
Gasoline	0.11	gal	16.0	0.94	liter	0.037
Diesel	0.0030	gal	0.48	0.025	liter	0.0011
Internal Offgas use (1)						
From Oil	53.2	lb	1,483	53.2	kg	3.45
From Natural Gas	100	lb	2,841	100	kg	6.61
Recovered Energy	207	thousand Btu	207	482	MJ	0.48
Total Process			21,188			49.3
Transportation Energy						
Combination truck	57.9	ton-miles		186	tonne-km	
Diesel	0.61	gal	96.5	5.07	liter	0.22
Rail	127	ton-miles		407	tonne-km	
Diesel	0.31	gal	49.9	2.62	liter	0.12
Barge	414	ton-miles		1,331	tonne-km	
Diesel	0.33	gal	52.6	2.76	liter	0.12
Residual oil	1.10	gal	189	9.18	liter	0.44
Ocean freighter	1,123	ton-miles		3,614	tonne-km	
Diesel	0.21	gal	33.9	1.78	liter	0.079
Residual	1.92	gal	330	16.0	liter	0.77
Pipeline-natural gas	313	ton-miles		1,007	tonne-km	
Natural gas	216	cu ft	242	13.5	cu meter	0.56
Pipeline-petroleum products	221	ton-miles		710	tonne-km	
Electricity	4.81	kwh	49.3	10.6	kwh	0.11
Total Transportation			1,042			2.42

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table J-1

DATA FOR THE PRODUCTION
OF ACRYLONITRILE-BUTADIENE-STYRENE (ABS) RESIN
(Cradle-to-Resin)
(page 2 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Ammonia	0.10	lb	0.10	kg
Antimony	1.3E-06	lb	1.3E-06	kg
Arsenic	1.7E-07	lb	1.7E-07	kg
Benzene	0.061	lb	0.061	kg
Carbon Dioxide - Fossil	253	lb	253	kg
Carbon Monoxide	0.88	lb	0.88	kg
Carbon Tetrachloride	8.8E-07	lb	8.8E-07	kg
CFC 13 (Methane, trichlorofluoro-)	1.4E-05	lb	1.4E-05	kg
Chlorine	1.1E-04	lb	1.1E-04	kg
Chromium	4.4E-07	lb	4.4E-07	kg
Ethylbenzene	0.0072	lb	0.0072	kg
Ethylene Dibromide	2.7E-06	lb	2.7E-06	kg
HCFC-22	1.0E-04	lb	1.0E-04	kg
Hydrogen	0.0029	lb	0.0029	kg
Hydrogen Chloride	5.9E-07	lb	5.9E-07	kg
Hydrogen Cyanide	0.010	lb	0.010	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.44	lb	0.44	kg
Methane	6.82	lb	6.82	kg
Nickel	3.7E-06	lb	3.7E-06	kg
Nitrogen Oxides	0.96	lb	0.96	kg
Non-Methane Hydrocarbons	2.15	lb	2.15	kg
Other Organics	0.14	lb	0.14	kg
Particulates (PM10)	0.094	lb	0.094	kg
Particulates (PM2.5)	0.020	lb	0.020	kg
Particulates (unspecified)	0.16	lb	0.16	kg
Polyaromatic Hydrocarbons (total)	3.6E-05	lb	3.6E-05	kg
Sulfur Dioxide	1.35	lb	1.35	kg
Sulfur Oxides	0.24	lb	0.24	kg
Toluene	0.093	lb	0.093	kg
VOC	0.49	lb	0.49	kg
Xylene	0.054	lb	0.054	kg
Solid Wastes				
Landfilled	52.4	lb	52.4	kg
Burned	7.29	lb	7.29	kg
Waste-to-Energy	0.81	lb	0.81	kg
Waterborne Wastes				
m-Xylene	8.8E-06	lb	8.8E-06	kg
1-Methylfluorene	1.6E-08	lb	1.6E-08	kg
2,4-Dimethylphenol	8.6E-06	lb	8.6E-06	kg
2-Hexanone	2.0E-06	lb	2.0E-06	kg
2-Methylnaphthalene	4.7E-06	lb	4.7E-06	kg
4-Methyl-2-Pentanone	5.9E-07	lb	5.9E-07	kg
Acetone	1.4E-06	lb	1.4E-06	kg
Acid (benzoic)	3.1E-04	lb	3.1E-04	kg
Acid (hexanoic)	6.4E-05	lb	6.4E-05	kg
Alkylated benzenes	5.8E-05	lb	5.8E-05	kg
Alkylated fluorenes	3.4E-06	lb	3.4E-06	kg
Alkylated naphthalenes	9.5E-07	lb	9.5E-07	kg
Alkylated phenanthrenes	3.9E-07	lb	3.9E-07	kg
Aluminum	0.028	lb	0.028	kg
Ammonia	0.12	lb	0.12	kg
Antimony	1.8E-05	lb	1.8E-05	kg
Arsenic	6.0E-05	lb	6.0E-05	kg
Barium	0.38	lb	0.38	kg
Benzene	3.4E-04	lb	3.4E-04	kg
Beryllium	3.8E-06	lb	3.8E-06	kg
BOD	0.37	lb	0.37	kg
Boron	9.6E-04	lb	9.6E-04	kg
Bromide	0.039	lb	0.039	kg
Cadmium	9.3E-06	lb	9.3E-06	kg
Calcium	0.65	lb	0.65	kg
Chlorides	7.95	lb	7.95	kg

Table J-1

DATA FOR THE PRODUCTION
OF ACRYLONITRILE-BUTADIENE-STYRENE (ABS) RESIN
(Cradle-to-Resin)
(page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Chromium (unspecified)	7.6E-04	lb	7.6E-04	kg
Cobalt	6.8E-06	lb	6.8E-06	kg
COD	3.83	lb	3.83	kg
Copper	8.3E-05	lb	8.3E-05	kg
Cyanide	1.0E-08	lb	1.0E-08	kg
Dibenzofuran	2.7E-08	lb	2.7E-08	kg
Dibenzothiophene	2.2E-08	lb	2.2E-08	kg
Dissolved Solids	9.22	lb	9.22	kg
Ethylbenzene	7.0E-04	lb	7.0E-04	kg
Fluorene	1.6E-06	lb	1.6E-06	kg
Iron	0.053	lb	0.053	kg
Lead	1.6E-04	lb	1.6E-04	kg
Lead 210	3.2E-14	lb	3.2E-14	kg
Lithium	0.095	lb	0.095	kg
Magnesium	0.13	lb	0.13	kg
Manganese	1.9E-04	lb	1.9E-04	kg
Mercury	3.5E-07	lb	3.5E-07	kg
Metal Ion (unspecified)	1.0E-04	lb	1.0E-04	kg
Methyl Chloride	5.6E-09	lb	5.6E-09	kg
Methyl Ethyl Ketone	1.1E-08	lb	1.1E-08	kg
Molybdenum	7.0E-06	lb	7.0E-06	kg
Naphthalene	5.5E-06	lb	5.5E-06	kg
n-Decane	8.8E-06	lb	8.8E-06	kg
n-Docosane	1.5E-07	lb	1.5E-07	kg
n-Dodecane	1.7E-05	lb	1.7E-05	kg
n-Eicosane	4.6E-06	lb	4.6E-06	kg
n-Hexacosane	9.4E-08	lb	9.4E-08	kg
n-Hexadecane	1.8E-05	lb	1.8E-05	kg
Nickel	7.2E-05	lb	7.2E-05	kg
Nitrates	0.010	lb	0.010	kg
n-Octadecane	4.6E-06	lb	4.6E-06	kg
p -Xylene	3.3E-06	lb	3.3E-06	kg
o -Xylene	3.3E-06	lb	3.3E-06	kg
o-Cresol	8.8E-06	lb	8.8E-06	kg
Oil	0.14	lb	0.14	kg
Other Organics	1.0E-04	lb	1.0E-04	kg
p-Cresol	9.5E-06	lb	9.5E-06	kg
p-Cymene	1.4E-08	lb	1.4E-08	kg
Pentamethylbenzene	1.1E-08	lb	1.1E-08	kg
Phenanthrene	2.4E-07	lb	2.4E-07	kg
Phenol/ Phenolic Compounds	9.7E-04	lb	9.7E-04	kg
Phosphates	0.010	lb	0.010	kg
Tetradecane	7.1E-06	lb	7.1E-06	kg
Radium 226	1.1E-11	lb	1.1E-11	kg
Radium 228	5.6E-14	lb	5.6E-14	kg
Selenium	4.5E-06	lb	4.5E-06	kg
Silver	3.9E-04	lb	3.9E-04	kg
Sodium	1.87	lb	1.87	kg
Strontium	0.017	lb	0.017	kg
Styrene	6.7E-04	lb	6.7E-04	kg
Sulfates	0.013	lb	0.013	kg
Sulfides	6.5E-04	lb	6.5E-04	kg
Sulfur	7.5E-04	lb	7.5E-04	kg
Surfactants	1.6E-04	lb	1.6E-04	kg
Suspended Solids	4.33	lb	4.33	kg
Thallium	3.7E-06	lb	3.7E-06	kg
Tin	7.0E-05	lb	7.0E-05	kg
Titanium	2.7E-04	lb	2.7E-04	kg
TOC	7.4E-04	lb	7.4E-04	kg
Toluene	3.8E-04	lb	3.8E-04	kg
Total biphenyls	3.7E-06	lb	3.7E-06	kg
Total dibenzothiophenes	1.2E-08	lb	1.2E-08	kg
Vanadium	4.3E-05	lb	4.3E-05	kg
Xylene, unspecified	1.5E-04	lb	1.5E-04	kg
Yttrium	2.0E-06	lb	2.0E-06	kg
Zinc	7.4E-04	lb	7.4E-04	kg

References: Tables B-2 through B-6, E-2, G-2, G-3, G-4, H-2, H-3, J-2, and J-3.

Source: Franklin Associates, A Division of ERG models

Table J-2

DATA FOR THE PRODUCTION OF AMMONIA

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Processed Natural Gas	267	lb		267	kg	
Water (as steam)	403	lb		403	kg	
Nitrogen (from air)	418	lb		418	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	63.5	kwh	653	140	kwh	1.52
Natural gas	2,239	cu ft	2,508	140	cu meters	5.84
Total Process			3,161			7.36
Transportation Energy						
Rail	125	ton-miles		402	tonne-km	
Diesel	0.31	gal	49.2	2.59	liter	0.11
Pipeline-petroleum products	1.25	ton-miles		4.02	tonne-km	
Electricity	0.027	kwh	0.28	0.060	kwh	6.5E-04
Total Transportation			49.5			0.12
Environmental Emissions						
Atmospheric Emissions						
Ammonia	1.00	lb		1.00	kg	
Other Organics	1.00	lb		1.00	kg	
Fossil Carbon Dioxide	97.0	lb		97.0	kg	
Solid Wastes						
Landfilled	0.20	lb		0.20	kg	
Waterborne Wastes						
Ammonia	0.060	lb		0.060	kg	
BOD	0.050	lb		0.050	kg	
COD	0.23	lb		0.23	kg	
Oil	0.050	lb		0.050	kg	
Suspended solids	0.050	lb		0.050	kg	

References: J-2 through J-5

Source: Franklin Associates, A Division of ERG

The energy and emissions data for acrylonitrile production is from a confidential source and is not shown to protect its confidentiality (Reference J-6). The company provided ranges for the material inputs and coproducts. The median of these ranges was used in the acrylonitrile dataset. Hydrogen cyanide and acetonitrile are produced as coproducts during this process. A mass basis was used to partition the credit for these coproducts. Waterborne emissions from the confidential dataset collected for acrylonitrile are sent to deepwell disposal, which is not included in this analysis, as the emissions are not released to a water source.

ABS Production

The two standard technologies for ABS production in North America are suspension or mass polymerization. Both of these technologies are represented within the ABS production dataset.

ABS is produced by grafting styrene and acrylonitrile onto a polybutadiene matrix. The three basic steps in the suspension process are: prepolymerization, polymerization, and product separation. The processing steps for mass polymerization are: prepolymerization, polymerization, devolatilization, and extrusion. Mass polymerization generates a minimum of wastewater and eliminates the need for dewatering and drying. In both the suspension and mass processes the polybutadiene must be soluble in styrene. Polybutadiene resin may be added as a dry resin rather than a latex.

Table J-3 presents the data for the production of ABS resin. Data for the production of ABS were provided by three leading producers (5 plants) in North America to Franklin Associates under contract to Plastics Division of the American Chemistry Council (ACC). Scrap and heat are produced as coproducts during this process. A mass basis was used to partition the credit for scrap, while the energy amount for the heat is reported separately as recovered energy.

As of 2003 there were 4 ABS producers and 7 ABS plants in the U.S. (Reference J-7). The ABS data collected represents a majority of the total North American ABS production amount. The ABS producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American ABS production. The average dataset was reviewed and accepted by all ABS data providers.

To assess the quality of the data collected for ABS, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for ABS include direct measurements and information provided by purchasing and utility records. All data submitted for ABS ranges from 2003-2004 and represents U.S. and Mexican production.

Table J-3

DATA FOR THE PRODUCTION OF ACRYLONITRILE-BUTADIENE-STYRENE (ABS)

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Ammonia	98	lb			98	kg	
Styrene	672	lb			672	kg	
Polybutadiene	144	lb			144	kg	
Water Consumption	314	gal			2,620	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	296	kwh		3,046	653	kwh	7.09
Electricity (cogeneration)	124	cu ft	(1)	139	7.73	cu meters	0.32
Natural gas	751	cu ft		841	46.9	cu meters	1.96
Bit./Sbit. Coal	68.4	lb		768	68.4	kg	1.79
Residual oil	0.045	gal		7.72	0.38	liter	0.018
Recovered Energy	204	thousand Btu		204	1,699	GJ	0.47
Total Process				4,598			10.7
Environmental Emissions							
Atmospheric Emissions							
Carbon Monoxide	0.010	lb	(2)		0.010	kg	
NM Hydrocarbons	0.12	lb			0.12	kg	
Nitrogen Oxides	0.010	lb	(2)		0.010	kg	
HCFC-22	1.0E-04	lb	(2)		1.0E-04	kg	
Other Organics	0.036	lb			0.036	kg	
Particulates	0.11	lb			0.11	kg	
Solid Wastes							
Landfilled	13.7	lb			13.7	kg	
Burned	2.29	lb			2.29	kg	
Waste-to-Energy	0.80	lb			0.80	kg	
Waterborne Wastes							
Ammonia	0.10	lb	(2)		0.10	kg	
BOD	0.010	lb	(2)		0.010	kg	
COD	2.91	lb			2.91	kg	
Dissolved solids	1.00	lb	(2)		1.00	kg	
Metal Ion	1.0E-04	lb	(2)		1.0E-04	kg	
Nitrates	0.010	lb	(2)		0.010	kg	
Oil	0.10	lb	(2)		0.10	kg	
Other Organics	1.0E-04	lb	(2)		1.0E-04	kg	
Phosphates	0.010	lb	(2)		0.010	kg	
Suspended solids	0.98	lb			0.98	kg	
Zinc	1.0E-04	lb	(2)		1.0E-04	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

Reference: J-8

Source: Franklin Associates, A Division of ERG

REFERENCES

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APPENDIX K

POLYETHER POLYOL FOR RIGID FOAM POLYURETHANE

INTRODUCTION

This appendix discusses the manufacture of the polyether polyol used for rigid foam polyurethanes. Examples of uses of rigid foam polyurethanes are insulation, packaging, and aviation. Over 200 million pounds of polyether polyols for use in rigid foam polyurethanes were produced in the U.S. and Canada in 2002 (Reference K-1). The material flow for this polyether polyol is shown in Figure K-1. The total unit process energy and emissions data (cradle-to-polyol) for this polyether polyol are displayed in Table K-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following processes are included in this appendix:

- Limestone Mining
- Sugar Beet Cultivation and Harvesting
- Sucrose Production
- Propylene Oxide Production
- Polyether Polyol for Rigid Foam Polyurethane

Crude oil production, distillation, desalting, and hydrotreating, natural gas production, and natural gas processing are discussed in Appendix B. Propylene production is discussed in Appendix E. Acetic acid production and oxygen production are discussed in Appendix F. Salt mining and sodium hydroxide/chlorine production are discussed in Appendix I.

Limestone Mining

Limestone is composed mainly of calcium carbonate in the form of the mineral calcite. It is quarried primarily from open pits. The most economical method of recovering the limestone is through blasting, followed by mechanical crushing and screening.

Particulate emissions arise from limestone crushing and screening operations (Reference K-3). Based on the type of technologies employed for limestone mining and processing, it is assumed that the release of other air emissions or water effluents is negligible (Reference K-4 and K-5).

Any overburden or tailings produced from limestone mining and processing are assumed to be returned to the mine site (References K-4 and K-5) and are not reported as solid waste.

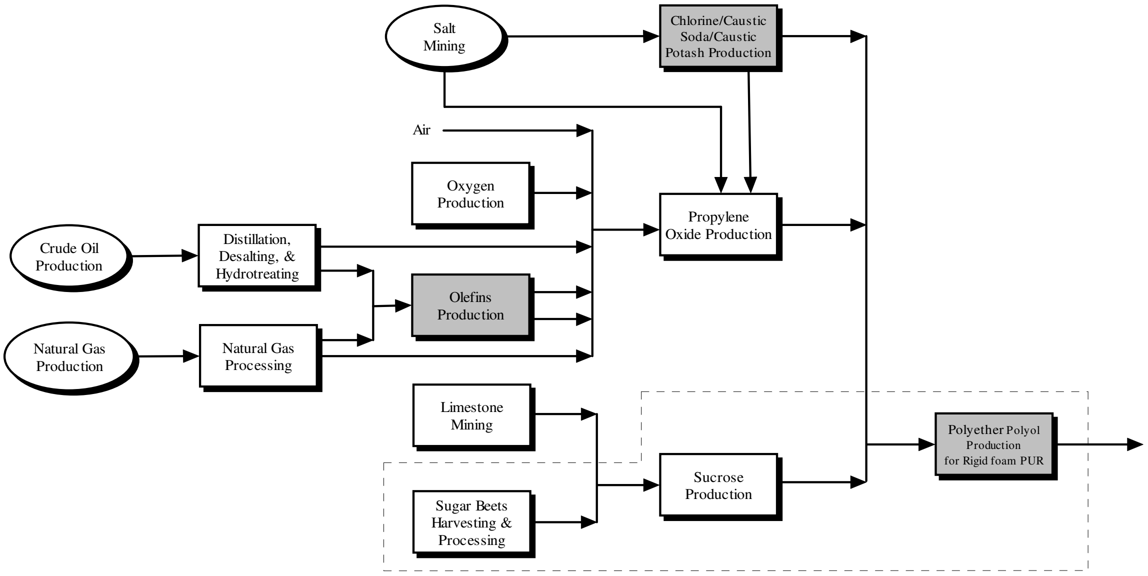

Figure K-1. Flow diagram for the manufacture of polyether polyol for rigid foam polyurethane. Shaded boxes represent partial or complete data provided by manufacturers specifically for this analysis. Boxes within the dotted lines are included in an aggregated dataset. Polyol types vary greatly by use. Additives are not included in this analysis of polyether polyols.

The energy requirements and environmental emissions for the mining and processing of limestone are shown in Table K-2.

Sugar Beet Cultivation and Harvesting

The sugar beet is a rotational crop, which requires nearly 4 times the land area of the equivalent cane crop (Reference K-6). Sugar beets are planted in the early spring. Agricultural practices include the application of fertilizer and pre-emergence herbicide at the time of planting. During the growing season, post-emergence herbicide is frequently applied as weeds can easily take away the water and nutrients from the soil. The root of the sugar beet plant is harvested in the fall, after a growing period of 120 to 200 days depending on the climate. The farmers defoliate the beets, then harvest them. Dirt is removed by shaking the beets using rollers on the way to the harvesting bin. The sugar beets are transported to a processing plant to where sucrose is produced.

The energy and emissions data for sugar beet cultivation and harvesting are from secondary sources. This dataset has been included with the polyether polyol average dataset (Table K-4) to conceal the confidential data of the limited number of provider companies.

Table K-1

DATA FOR THE PRODUCTION OF POLYETHER POLYOL FOR RIGID FOAM POLYURETHANES

(Cradle-to-Polyol)

(page 1 of 3)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	214	lb		214	kg	
Natural Gas	380	lb		380	kg	
Salt	1,565	lb		1,565	kg	
Sugar Beets	1,215	lb		1,215	kg	
Limestone	72.5	lb		72.5	kg	
Oxygen	74.9	lb		74.9	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			8,133			18.9
Petroleum			4,008			9.33
Total Resource			12,140			28.3
Process Energy						
Electricity (grid)	532	kwh	5,655	1,172	kwh	13.2
Electricity (cogeneration)	1,495	cu ft (2)	1,674	93.3	cu meters	3.90
Natural gas	6,942	cu ft	7,775	433	cu meters	18.1
LPG	0.035	gal	3.76	0.29	liter	0.0088
Bit./Sbit. Coal	97.0	lb	1,089	97.0	kg	2.54
Distillate oil	2.01	gal	319	16.7	liter	0.74
Residual oil	13.0	gal	2,224	108	liter	5.18
Gasoline	3.10	gal	441	25.9	liter	1.03
Diesel	1.82	gal	289	15.2	liter	0.67
Internal Offgas use (1)						
From Oil	38.9	lb	1,107	38.9	kg	2.58
From Natural Gas	69.2	lb	1,968	69.2	kg	4.58
Recovered Energy	101	thousand Btu	101	234	MJ	0.23
Total Process			22,443			52.2
Transportation Energy						
Combination truck	150	ton-miles		483	tonne-km	
Diesel	1.58	gal	250	13.2	liter	0.58
Rail	36.5	ton-miles		117	tonne-km	
Diesel	0.090	gal	14.4	0.75	liter	0.033
Barge	21.3	ton-miles		68.6	tonne-km	
Diesel	0.017	gal	2.71	0.14	liter	0.0063
Residual oil	0.057	gal	9.73	0.47	liter	0.023
Ocean freighter	373	ton-miles		1,199	tonne-km	
Diesel	0.071	gal	11.2	0.59	liter	0.026
Residual	0.64	gal	109	5.32	liter	0.25
Pipeline-natural gas	224	ton-miles		719	tonne-km	
Natural gas	154	cu ft	173	9.62	cu meter	0.40
Pipeline-petroleum products	266	ton-miles		857	tonne-km	
Electricity	5.81	kwh	59.5	12.8	kwh	0.14
Total Transportation			630			1.47

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table K-1

DATA FOR THE PRODUCTION OF POLYETHER POLYOL FOR RIGID FOAM POLYURETHANES

(Cradle-to-Polyol)

(page 2 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Acid (unknown)	0.033	lb	0.033	kg
Ammonia	0.038	lb	0.038	kg
Antimony	5.1E-07	lb	5.1E-07	kg
Arsenic	6.4E-08	lb	6.4E-08	kg
Benzene	0.043	lb	0.043	kg
Carbon Dioxide - Fossil	58.3	lb	58.3	kg
Carbon Monoxide	0.24	lb	0.24	kg
Carbon Tetrachloride	1.8E-04	lb	1.8E-04	kg
CFC 13 (Methane, trichlorofluoro-)	5.4E-06	lb	5.4E-06	kg
Chlorine	0.0022	lb	0.0022	kg
Chromium	1.7E-07	lb	1.7E-07	kg
Ethylbenzene	0.73	lb	0.73	kg
Ethylene Dibromide	1.1E-06	lb	1.1E-06	kg
HCFC-123	8.3E-05	lb	8.3E-05	kg
HCFC-22	5.9E-07	lb	5.9E-07	kg
HFC-134a	8.3E-05	lb	8.3E-05	kg
Hydrogen	0.0030	lb	0.0030	kg
Hydrogen Chloride	2.9E-04	lb	2.9E-04	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.17	lb	0.17	kg
Lead	9.7E-09	lb	9.7E-09	kg
Mercury	1.6E-04	lb	1.6E-04	kg
Methane	3.72	lb	3.72	kg
Nickel	1.4E-06	lb	1.4E-06	kg
Nitrogen Oxides	0.53	lb	0.53	kg
Non-Methane Hydrocarbons	4.49	lb	4.49	kg
Other Organics	0.11	lb	0.11	kg
Particulates (PM10)	0.12	lb	0.12	kg
Particulates (PM2.5)	0.016	lb	0.016	kg
Particulates (unspecified)	0.26	lb	0.26	kg
Polyaromatic Hydrocarbons (total)	1.4E-05	lb	1.4E-05	kg
Propylene Oxide	0.36	lb	0.36	kg
Sulfur Dioxide	0.91	lb	0.91	kg
Sulfur Oxides	0.0039	lb	0.0039	kg
Toluene	0.067	lb	0.067	kg
VOC	0.35	lb	0.35	kg
Xylene	0.039	lb	0.039	kg
Solid Wastes				
Landfilled	21.3	lb	21.3	kg
Burned	4.57	lb	4.57	kg
Waste-to-Energy	0.0026	lb	0.0026	kg
Waterborne Wastes				
m-Xylene	5.0E-06	lb	5.0E-06	kg
1-Methylfluorene	1.0E-08	lb	1.0E-08	kg
2,4-Dimethylphenol	4.8E-06	lb	4.8E-06	kg
2-Hexanone	1.1E-06	lb	1.1E-06	kg
2-Methylnaphthalene	2.6E-06	lb	2.6E-06	kg
4-Methyl-2-Pentanone	3.8E-07	lb	3.8E-07	kg
Acetone	9.1E-07	lb	9.1E-07	kg
Acid (benzoic)	1.7E-04	lb	1.7E-04	kg
Acid (hexanoic)	3.6E-05	lb	3.6E-05	kg
Acid (unspecified)	7.56	lb	7.56	kg
Alkylated benzenes	3.2E-05	lb	3.2E-05	kg
Alkylated fluorenes	1.9E-06	lb	1.9E-06	kg
Alkylated naphthalenes	5.3E-07	lb	5.3E-07	kg
Alkylated phenanthrenes	2.2E-07	lb	2.2E-07	kg
Aluminum	0.016	lb	0.016	kg
Ammonia	0.0056	lb	0.0056	kg
Antimony	9.8E-06	lb	9.8E-06	kg
Arsenic	3.3E-05	lb	3.3E-05	kg
Barium	0.21	lb	0.21	kg
Benzene	1.9E-04	lb	1.9E-04	kg
Beryllium	2.1E-06	lb	2.1E-06	kg
BOD	1.16	lb	1.16	kg
Boron	5.3E-04	lb	5.3E-04	kg
Bromide	0.021	lb	0.021	kg
Cadmium	5.1E-06	lb	5.1E-06	kg
Calcium	0.35	lb	0.35	kg
Chlorides	4.37	lb	4.37	kg

Table K-1

DATA FOR THE PRODUCTION
OF POLYETHER POLYOL FOR RIGID FOAM POLYURETHANES
(Cradle-to-Polyol)
(page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Chromium (unspecified)	4.2E-04	lb	4.2E-04	kg
Cobalt	3.8E-06	lb	3.8E-06	kg
COD	1.09	lb	1.09	kg
Copper	4.6E-05	lb	4.6E-05	kg
Cyanide	6.5E-09	lb	6.5E-09	kg
Dibenzofuran	1.7E-08	lb	1.7E-08	kg
Dibenzothiophene	1.4E-08	lb	1.4E-08	kg
Dissolved Solids	44.3	lb	44.3	kg
Ethylbenzene	1.6E-05	lb	1.6E-05	kg
Fluorene	8.7E-07	lb	8.7E-07	kg
Hydrocarbons	0.70	lb	0.70	kg
Iron	0.029	lb	0.029	kg
Lead	8.7E-05	lb	8.7E-05	kg
Lead 210	1.8E-14	lb	1.8E-14	kg
Lithium	0.067	lb	0.067	kg
Magnesium	0.071	lb	0.071	kg
Manganese	1.0E-04	lb	1.0E-04	kg
Mercury	6.8E-07	lb	6.8E-07	kg
Methyl Chloride	3.6E-09	lb	3.6E-09	kg
Methyl Ethyl Ketone	7.3E-09	lb	7.3E-09	kg
Molybdenum	3.9E-06	lb	3.9E-06	kg
Naphthalene	3.1E-06	lb	3.1E-06	kg
n-Decane	4.9E-06	lb	4.9E-06	kg
n-Docosane	9.7E-08	lb	9.7E-08	kg
n-Dodecane	9.4E-06	lb	9.4E-06	kg
n-Eicosane	2.6E-06	lb	2.6E-06	kg
n-Hexacosane	6.0E-08	lb	6.0E-08	kg
n-Hexadecane	1.0E-05	lb	1.0E-05	kg
Nickel	4.0E-05	lb	4.0E-05	kg
Nitrogen	0.91	lb	0.91	kg
n-Octadecane	2.5E-06	lb	2.5E-06	kg
p -Xylene	1.8E-06	lb	1.8E-06	kg
o -Xylene	1.8E-06	lb	1.8E-06	kg
o-Cresol	4.9E-06	lb	4.9E-06	kg
Oil	0.0057	lb	0.0057	kg
p-Cresol	5.3E-06	lb	5.3E-06	kg
p-Cymene	9.0E-09	lb	9.0E-09	kg
Pentamethylbenzene	6.8E-09	lb	6.8E-09	kg
Phenanthrene	1.4E-07	lb	1.4E-07	kg
Phenol/ Phenolic Compounds	1.01	lb	1.01	kg
Tetradecane	4.0E-06	lb	4.0E-06	kg
Radium 226	6.2E-12	lb	6.2E-12	kg
Radium 228	3.2E-14	lb	3.2E-14	kg
Selenium	2.3E-06	lb	2.3E-06	kg
Silver	2.1E-04	lb	2.1E-04	kg
Sodium	1.01	lb	1.01	kg
Sodium Hydroxide	1.08	lb	1.08	kg
Strontium	0.0093	lb	0.0093	kg
Styrene	5.9E-07	lb	5.9E-07	kg
Sulfates	0.0073	lb	0.0073	kg
Sulfides	9.0E-05	lb	9.0E-05	kg
Sulfur	4.2E-04	lb	4.2E-04	kg
Surfactants	8.6E-05	lb	8.6E-05	kg
Suspended Solids	1.82	lb	1.82	kg
Thallium	2.1E-06	lb	2.1E-06	kg
Tin	3.9E-05	lb	3.9E-05	kg
Titanium	1.5E-04	lb	1.5E-04	kg
TOC	5.9E-04	lb	5.9E-04	kg
Toluene	2.3E-04	lb	2.3E-04	kg
Total biphenyls	2.1E-06	lb	2.1E-06	kg
Total dibenzothiophenes	6.4E-09	lb	6.4E-09	kg
Vanadium	1.8E-05	lb	1.8E-05	kg
Xylene, unspecified	8.0E-05	lb	8.0E-05	kg
Yttrium	1.1E-06	lb	1.1E-06	kg
Zinc	3.6E-04	lb	3.6E-04	kg

References: Tables B-2 through B-6, E-2, F-4, I-2, I-3b, K-2, K-3, and K-4.

Source: Franklin Associates, A Division of ERG models

Table K-2

DATA FOR THE MINING AND PROCESSING OF LIMESTONE

	English units (Basis: 1,000 lb)		Total Energy Thousand Btu	SI units (Basis: 1,000 kg)		Total Energy GigaJoules
Energy Usage						
Process Energy						
Electricity (grid)	1.92	kwh	19.8	4.23	kwh	0.046
Natural gas	2.25	cu ft	2.52	0.14	cu meters	0.0059
Bit./Sbit. Coal	0.036	lb	0.40	0.036	kg	9.4E-04
Distillate oil	0.070	gal	11.1	0.58	liter	0.026
Gasoline	0.0061	gal	0.87	0.051	liter	0.0020
Total Process			34.7			0.081
Transportation Energy						
Combination truck	21.0	ton-miles		67.6	tonne-km	
Diesel	0.22	gal	35.0	1.84	liter	0.081
Rail	5.00	ton-miles		16.1	tonne-km	
Diesel	0.012	gal	1.97	0.10	liter	0.0046
Barge	13.0	ton-miles		41.8	tonne-km	
Diesel	0.010	gal	1.65	0.087	liter	0.0038
Residual oil	0.035	gal	5.93	0.29	liter	0.014
Total Transportation			44.6			0.10
Environmental Emissions						
Atmospheric Emissions						
Particulates (unknown)	0.051	lb		0.051	kg	

References: K-2 through K-5

Source: Franklin Associates, A Division of ERG

Sucrose Production

Sucrose is commonly produced from sugar cane and sugar beets. For this project, sucrose production is based on production from sugar beets. Both cane and beet sucrose are produced in North America and could be used for this purpose. Other principal products of sugar beet processing are molasses and beet pulp. These have been given coproduct credit on a mass basis.

When the beets arrive to be processed into granulated sugar, they are washed, sliced, and weighed. Significant amounts of soil associated with the incoming beets are removed here, as well as beet tops and other organic matter; these are commonly land applied. The sliced beets are fed to a counter-current diffuser where sugar and other soluble materials are dissolved from the beets. From the diffuser, the beet slices are pressed in screw presses to squeeze as much juice as possible from them. The "raw juice" is carbonated and clarified by adding milk of lime (CaOH) and carbon dioxide. The juice is then thickened in multiple effect evaporators and crystallized in vacuum pans to obtain sugar. The sugar is centrifuged to separate it from adhering syrup, and then dried. In many beet processing plants, a Steffan process has been added to further extract sugar from molasses. This process increases the sugar yield while reducing the molasses output, but also increases the limestone requirements (Reference K-6).

Energy requirements and environmental emissions for sucrose production are from a 1991 European confidential source, which was reviewed and updated in 2005 by an expert in the U.S. sucrose industry. The energy requirements, solid waste, and atmospheric emissions were edited to represent the current U.S. sucrose industry.

The sucrose dataset has been included with the polyether polyol average dataset (Table K-4) to conceal the confidential data of all provider companies.

Propylene Oxide Production

Two different processes for the production of propylene oxide are currently in use. These are the chlorohydrin process and hydroperoxidation processes, using either ethylbenzene, isobutene, or MTBE. The MTBE hydroperoxidation process is approximately the same as the isobutene hydroperoxidation process. The chlorohydrin process is the oldest and is less flexible because it produces only propylene oxide. The hydroperoxide reactions, however, produce marketable co-products in addition to propylene oxide.

The data in Table K-3 represent the energy requirements and environmental emissions for the production of propylene oxide. The energy requirements are based on data in a Department of Energy report from 2000 (Reference K-7). No information was given in the DoE report about the technology or mix of technologies represented by the energy data. The environmental emissions and raw materials are based on three datasets from a confidential secondary source. These amounts are a weighted average of the three technologies based on 2001 capacity. The chlorohydrin process generates 42.1 percent of the propylene oxide, the isobutene hydroperoxidation (including MTBE hydroperoxidation) 34.6 percent, and the ethylbenzene hydroperoxidation 23.3 percent (Reference K-8). In the two hydroperoxidation datasets, coproduct credit was given on a mass basis.

The chlorohydrin process begins with a equal molar mixture of propylene and chlorine in water, which forms the solution propylene chlorohydrin. The chlorohydrin solution is treated with a base, usually cell liquor from a chlorine plant, to form the oxide. Propylene oxide is then stripped from the alkaline solution and purified by distilling the light ends, then the oxide.

In the isobutene hydroperoxide process, propylene oxide and tert-butyl alcohol are formed from isobutene, oxygen, and propylene. Isobutane is first oxidized to the intermediate, tert-butyl hydroperoxide. This intermediate and an alcohol mixture coproduct is combined with propylene. This is reacted to nearly 100 percent conversion of the hydroperoxide over a catalyst. The products stream contains propylene oxide and tert-butyl alcohol. The products are separated in distillation columns.

Table K-3

DATA FOR THE PRODUCTION OF PROPYLENE OXIDE

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Propylene	773	lb		773	kg	
Chlorine	573	lb		573	kg	
Sodium Hydroxide	689	lb		689	kg	
Sodium Chloride	928	lb		928	kg	
Oxygen	98.6	lb		98.6	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	128	kwh	1,322	283	kwh	3.08
Natural gas	2,328	cu ft	2,607	145	cu meters	6.07
Residual oil	15.7	gal	2,692	131	liter	6.27
Total Process			6,621			15.4
Transportation Energy						
Used in polyether polyols for rigid foam PUR						
Combination truck	50.0	ton-miles		161	tonne-km	
Diesel	0.53	gal	83.4	4.38	liter	0.19
Pipeline-petroleum products	0.50	ton-miles		1.61	tonne-km	
Electricity	0.011	kwh	0.11	0.024	kwh	2.6E-04
Total Transportation			83.5			0.19
Used in polyether polyols for flexible foam PUR						
Combination truck	4.57	ton-miles		14.7	tonne-km	
Diesel	0.048	gal	7.62	0.40	liter	0.018
Rail	9.39	ton-miles		30.2	tonne-km	
Diesel	0.023	gal	3.70	0.19	liter	0.0086
Pipeline-petroleum products	0.40	ton-miles		1.29	tonne-km	
Electricity	0.0087	kwh	0.089	0.019	kwh	2.1E-04
Total Transportation			11.4			0.027
Environmental Emissions						
Atmospheric Emissions						
Acid (unknown)	0.044	lb		0.044	kg	
Ammoina	0.049	lb		0.049	kg	
Carbon Dioxide	12.8	lb		12.8	kg	
Chlorine	0.0013	lb		0.0013	kg	
Ethylbenzene	0.96	lb		0.96	kg	
Hydrocarbons	5.83	lb		5.83	kg	
Propylene Oxide	0.47	lb		0.47	kg	
Solid Wastes						
Landfilled	0.20	lb		0.20	kg	
Waterborne Wastes						
Acid (unknown)	9.95	lb		9.95	kg	
Hydrocarbons	0.92	lb		0.92	kg	
Phenol	1.33	lb		1.33	kg	
Sodium Hydroxide	1.42	lb		1.42	kg	

References: K-7 through K-9.

Source: Franklin Associates, A Division of ERG

In the ethylbenzene hydroperoxide reaction, propylene oxide and styrene are produced. Ethylbenzene and oxygen are reacted to form ethylbenzene hydroperoxide and small amounts of methylbenzyl alcohol and acetophenone. This solution and propylene are fed to the epoxidation reactor. The products stream contains propylene oxide, propylene, methylbenzyl alcohol, and small amounts of several other hydrocarbons. Propylene oxide is purified by a multi-tower distillation scheme.

Polyether Polyol Production for Rigid Foam Polyurethane

The manufacturing of the polyether polyol used in rigid foam polyurethane production begins with the introduction of a potassium hydroxide catalyst to an initiator. In this analysis, sucrose was chosen as the initiator; however, glycerine and sorbitol are also common initiators used to produce polyether polyols for rigid foam polyurethane. This solution is then reacted with propylene oxide to form an intermediate. The catalyst is removed using an acid, which produces a salt that must be filtered. This acid amount is small and considered negligible in this analysis. Finally, the polyol is purified of side products and water through distillation. Sodium hydroxide data is used in place of potassium hydroxide data which were not available. The manufacture of sodium hydroxide utilizes a process similar to the manufacture of potassium hydroxide.

Table K-4 presents the data for the production of polyether polyol for use in rigid foam polyurethane. Data for the production of polyether polyol were provided by two leading producers (2 plants) in North America to Franklin Associates under contract to Plastics Division of the American Chemistry Council (ACC). Heat was a coproduct for one producer. The energy for exported heat was reported separately as recovered energy.

As of 2002, it is estimated that for all polyurethane applications, there were 7 polyether polyol producers and 9 polyether polyol plants in the U.S. (Reference K-1 and K-18). The polyether polyol data collected represents a majority of the total North American production of polyether polyol for rigid foam polyurethane. The polyether polyol producers who provided data for this module verified that the characteristics of their plants are representative of a majority of the North American production. The average dataset was reviewed and accepted by both polyether polyol data providers.

To assess the quality of the data collected for polyether polyols in rigid foam polyurethane, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for these polyether polyols include direct measurements, information provided by purchasing and utility records, and engineering estimates. All data submitted for polyether polyols represents the year 2003 and represents U.S. production.

Table K-4

DATA FOR THE PRODUCTION OF POLYETHER POLYOLS FOR RIGID FOAM POLYURETHANES

(includes sugar beet harvesting/processing and sucrose production)

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Propylene oxide	760	lb			760	kg	
Potassium hydroxide	13.0	lb			13.0	kg	
Limestone	72.5	lb			72.5	kg	
Sugar beets	1,215	lb			1,215	kg	
Water Consumption	0.5	gal			4.17	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	48.3	kwh		497	106	kwh	1.16
Electricity (cogeneration)	401	cu ft	(1)	449	25.0	cu meters	1.05
Natural gas	1,087	cu ft		1,217	67.9	cu meters	2.83
Bit./Sbit. Coal	54.4	lb		611	54.4	kg	1.42
Gasoline	3.04	gal		432	25.4	liter	1.01
Diesel	1.82	gal		289	15.2	liter	0.67
Recovered Energy	98.1	thousand Btu		98.1	228	MJ	0.23
Total Process				3,398			7.91
Transportation Energy (2)							
Combination truck	39.5	ton-miles			127	tonne-km	
Diesel	0.41	gal		65.9	3.46	liter	0.15
Rail	9.72	ton-miles			31.3	tonne-km	
Diesel	0.024	gal		3.83	0.20	liter	0.0089
Total Transportation				69.7			0.16
Environmental Emissions							
Atmospheric Emissions							
Carbon Dioxide	16.8	lb			16.8	kg	
Carbon Monoxide	0.13	lb			0.13	kg	
Chlorine	1.0E-04	lb	(3)		1.0E-04	kg	
Nitrogen Oxides	0.42	lb			0.42	kg	
Other Organics	0.11	lb			0.11	kg	
Particulates (unknown)	0.25	lb			0.25	kg	
PM2.5	0.010	lb	(3)		0.010	kg	
PM10	0.033	lb			0.033	kg	
Sulfur Oxides	0.0010	lb			0.0010	kg	
Solid Wastes							
Landfilled	0.064	lb			0.064	kg	
Waterborne Wastes (4)							
BOD	0.89	lb			0.89	kg	
COD	1.00	lb	(3)		1.00	kg	
Nitrogen	0.91	lb			0.91	kg	
Suspended solids	1.0.E-04	lb	(3)		1.0E-04	kg	

---

(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) Transportation energy represents transporting the sugar beets to the sucrose plant and the sucrose to the polyols plant.

(3) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(4) These waterborne emissions may be overstated as 1 or more of the plants providing data were only able to supply waterborne emissions before the effluent was sent to a water treatment plant.

References: K-11 through K-17.

Source: Franklin Associates, A Division of ERG

REFERENCES

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K-2. **Energy and Environmental Profile of the U.S. Mining Industry.** U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy. December 2002.

K-3. **AP-42 Emission Factors. Chapter 11.19.2.** Crushed Stone Processing and Pulverized Mineral Processing. US EPA. August 2004.

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K-6. Information compiled from the website: http://www.sucrose.com/lbeet.html

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K-8. Chemical profiles information taken from the website: http://www.the-innovation-group.com/welcome.htm.

K-9. Data compiled by Franklin Associates, based on a confidential secondary source. 1993.

K-10. Polyurethane 102, Polyurethane Chemistry and Raw Materials. Slides and notes from the Polyurethane Professional Development Program produced by the Alliance for the Polyurethanes Industry. 2003 edition.

K-11. Franklin Associates estimate.

K-12. Data taken from the report **Resource and Environmental Profile Analysis of Three Methods of Manufacturing Liquid Sweeteners** performed by Midwest Research Institute. 1974.

K-13. Personal communication between Franklin Associates and Paul Fry of Fry Engineering, consultant to the sucrose industry. 2005.

K-14. Calculations based on estimates given by Paul Fry of Fry Engineering, consultant to the sucrose industry. 2005.

K-15. Calculations performed by Paul Fry of Fry Engineering, consultant to the sucrose industry. 2005.

K-16. Data compiled by Franklin Associates, Ltd., based on contact with a confidential European source. 1991.

K-17. Information and data collected from APC member and non-member companies producing polyether polyol for rigid foam polyurethane. 2003.

K-18. Research by Franklin Associates on each polyol producing companies' website.

APPENDIX L

POLYETHER POLYOL FOR FLEXIBLE FOAM POLYURETHANE

INTRODUCTION

This appendix discusses the manufacture of the polyether polyol used for flexible foam polyurethanes. Examples of uses of flexible foam polyurethanes are furniture, carpet underlay, and automotive seats. Over 1.2 billion pounds of polyether polyols used in flexible foam polyurethanes were produced in the U.S. and Canada in 2002 (Reference L-1). The material flow for this polyether polyol is shown in Figure L-1. The total unit process energy and emissions data (cradle-to-polyol) for this polyether polyol are displayed in Table L-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. Processes that have been discussed in a previous appendix have been omitted from this appendix. The following processes are included in this appendix:

- Fresh fruit bunch harvesting
- Palm kernels production
- Palm kernel oil processing
- Palm kernel oil refining, bleaching and deodorizing
- Glycerine production
- Polyether polyol for flexible foam polyurethane

Crude oil production, distillation, desalting, and hydrotreating, natural gas production, natural gas processing, and ethylene production are discussed in Appendix B. Propylene production is discussed in Appendix E. Ethylene oxide production, methanol production, and oxygen production are discussed in Appendix F. Salt mining and sodium hydroxide/chlorine production are discussed in Appendix I. Propylene oxide production is discussed in Appendix K.

Fresh Fruit Bunch Harvesting

With an average rainfall of 210 centimeters per year, an average temperature of 85° to 90° Fahrenheit, and the generally flat geographic terrain, Malaysia is ideal for growing palm trees for palm oil production. A palm tree produces its first harvest between the ages of 30 and 36 months. Once the tree begins producing fruit it may be harvested every 10 to 21 days for the remainder of its life (approximately 25 years) (Reference L-2).

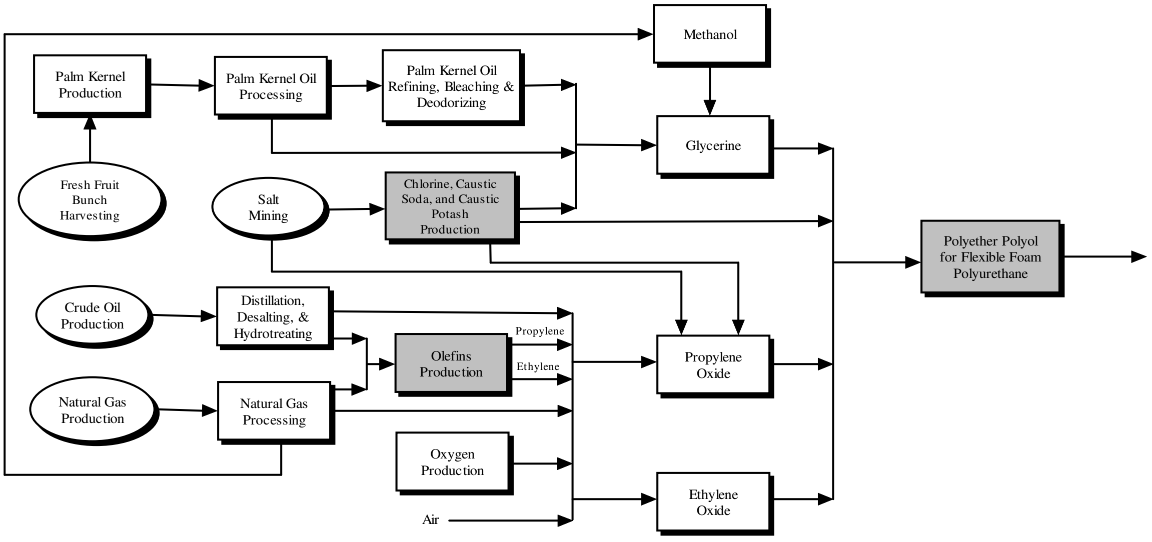

Figure L-1. Flow diagram for the manufacture of polyether polyol for flexible foam polyurethane. Shaded boxes represent partial or complete data provided by manufacturers specifically for this analysis.

There are approximately 54 palm trees per acre, or 130 palm trees per hectare (Reference L-3). An individual palm fruit is four centimeters long and grows in a cluster or bunch on the inner base of the palm frond. Therefore, in order to harvest a fresh fruit bunch (FFB), a palm frond must be manually cut from the tree. Once the frond has been removed, the stalk of the FFB falls to the ground. To prevent bruising of FFBs, harvesting crews typically catch the FFB before it hits the ground.

The FFB are then taken to one of the plantation's access roads where they are loaded into trucks or trailers and shipped to the palm oil mill for processing (Reference L-4). Less than 5 percent of the harvested FFB are transported to the mill by rail.

The energy required for harvesting comes from transporting FFB from the fields to the palm oil mill. Environmental emissions result primarily from burning of older trees on the plantation. Older trees are taken out of production in part because their height makes harvesting very difficult. At any given time, 10 percent of a plantation will be in the stages of replanting (Reference L-3).

The pruned palm fronds, as well as the fallen and burned tree, are utilized as soil conditioners or additives (Reference L-2). The pruned palm fronds are left on the ground under the palm tree as a mulch material and allowed to naturally degrade. It is not uncommon for palm oil mill effluent (POME), which is relatively high in potassium, phosphorus, and nitrogen, to be applied to the soil or fronds to aid in their degradation and act as a fertilizer. With the palm fronds and the resultant ash from burning the tree being utilized, the only emissions to report are the atmospheric emissions from burning the older palm trees.

Table L-1

DATA FOR THE PRODUCTION OF POLYETHER POLYOL FOR FLEXIBLE FOAM POLYURETHANES

(Cradle-to-Polyol)

(page 1 of 4)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Raw Materials						
Crude oil	257	lb		257	kg	
Natural Gas	504	lb		504	kg	
Salt	1,753	lb		1,753	kg	
Fresh Fruit Bunches	76.5	lb		76.5	kg	
Oxygen	184	lb		184	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			10,796			25.1
Petroleum			4,830			11.2
Total Resource			15,626			36.4
Process Energy						
Electricity (grid)	580	kwh	6,169	1,279	kwh	14.4
Electricity (cogeneration)	1,561	cu ft (2)	1,749	97.5	cu meters	4.07
Natural gas	8,110	cu ft	9,084	506	cu meters	21.1
LPG	0.042	gal	4.52	0.35	liter	0.011
Bit./Sbit. Coal	48.9	lb	549	48.9	kg	1.28
Distillate oil	2.41	gal	382	20.1	liter	0.89
Residual oil	14.7	gal	2,517	122	liter	5.86
Gasoline	0.079	gal	11.3	0.66	liter	0.026
Diesel	0.15	gal	24.1	1.27	liter	0.056
Biomass	97.6	thousand Btu	97.6	227	MJ	0.23
Internal Offgas use (1)						
From Oil	46.2	lb	1,318	46.2	kg	3.07
From Natural Gas	88.5	lb	2,541	88.5	kg	5.92
Recovered Energy	81.6	thousand Btu	81.6	190	MJ	0.19
Total Process			24,365			56.7
Transportation Energy						
Combination truck	85.0	ton-miles		274	tonne-km	
Diesel	0.89	gal	142	7.45	liter	0.33
Single unit truck	0.79	ton-miles		2.55	tonne-km	
Diesel	0.018	gal	2.83	0.15	liter	0.0066
Rail	40.8	ton-miles		131	tonne-km	
Diesel	0.10	gal	16.1	0.84	liter	0.037
Barge	24.4	ton-miles		78.6	tonne-km	
Diesel	0.020	gal	3.10	0.16	liter	0.0072
Residual oil	0.065	gal	11.1	0.54	liter	0.026
Ocean freighter	550	ton-miles		1,770	tonne-km	
Diesel	0.10	gal	16.6	0.87	liter	0.039
Residual	0.94	gal	161	7.85	liter	0.38
Pipeline-natural gas	295	ton-miles		950	tonne-km	
Natural gas	204	cu ft	228	12.7	cu meter	0.53
Pipeline-petroleum products	310	ton-miles		998	tonne-km	
Electricity	6.76	kwh	69.2	14.9	kwh	0.16
Total Transportation			650			1.51

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table L-1

DATA FOR THE PRODUCTION
OF POLYETHER POLYOL FOR FLEXIBLE FOAM POLYURETHANES

(Cradle-to-Polyol)

(page 2 of 4)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Acid (unknown)	0.038	lb	0.038	kg
Aldehydes (unspecified)	0.032	lb	0.032	kg
Ammonia	0.043	lb	0.043	kg
Antimony	6.1E-07	lb	6.1E-07	kg
Arsenic	7.7E-08	lb	7.7E-08	kg
Benzene	0.057	lb	0.057	kg
Carbon Dioxide - Fossil	147	lb	147	kg
Carbon Dioxide - Non-Fossil	16.9	lb	16.9	kg
Carbon Monoxide	0.16	lb	0.16	kg
Carbon Tetrachloride	2.0E-04	lb	2.0E-04	kg
CFC 13 (Methane, trichlorofluoro-)	6.5E-06	lb	6.5E-06	kg
Chlorine	0.0024	lb	0.0024	kg
Chromium	2.0E-07	lb	2.0E-07	kg
Ethylbenzene	0.83	lb	0.83	kg
Ethylene Dibromide	1.3E-06	lb	1.3E-06	kg
Ethylene Oxide	0.011	lb	0.011	kg
HCFC-123	9.2E-05	lb	9.2E-05	kg
HCFC-22	7.5E-07	lb	7.5E-07	kg
HFC-134a	9.2E-05	lb	9.2E-05	kg
Hydrogen	0.0038	lb	0.0038	kg
Hydrogen Chloride	3.3E-04	lb	3.3E-04	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.20	lb	0.20	kg
Lead	1.1E-07	lb	1.1E-07	kg
Mercury	1.7E-04	lb	1.7E-04	kg
Methane	5.69	lb	5.69	kg
Nickel	1.7E-06	lb	1.7E-06	kg
Nitrogen Oxides	0.20	lb	0.20	kg
Nitrous Oxide	1.0E-04	lb	1.0E-04	kg
Non-Methane Hydrocarbons	7.32	lb	7.32	kg
Odorous Sulfur	0.0039	lb	0.0039	kg
Other Organics	0.10	lb	0.10	kg
Particulates (PM10)	0.16	lb	0.16	kg
Particulates (PM2.5)	0.017	lb	0.017	kg
Particulates (unspecified)	0.092	lb	0.092	kg
Polyaromatic Hydrocarbons (total)	1.7E-05	lb	1.7E-05	kg
Propylene Oxide	0.40	lb	0.40	kg
Sulfur Dioxide	1.19	lb	1.19	kg
Sulfur Oxides	0.031	lb	0.031	kg
Toluene	0.088	lb	0.088	kg
VOC	0.46	lb	0.46	kg
Xylene	0.051	lb	0.051	kg
Solid Wastes				
Landfilled	30.9	lb	30.9	kg
Burned	5.46	lb	5.46	kg
Waste-to-Energy	0.0050	lb	0.0050	kg
Waterborne Wastes				
m-Xylene	6.4E-06	lb	6.4E-06	kg
1-Methylfluorene	1.3E-08	lb	1.3E-08	kg
2,4-Dimethylphenol	6.1E-06	lb	6.1E-06	kg
2-Hexanone	1.4E-06	lb	1.4E-06	kg
2-Methylnaphthalene	3.3E-06	lb	3.3E-06	kg
4-Methyl-2-Pentanone	5.0E-07	lb	5.0E-07	kg
Acetaldehyde	0.011	lb	0.011	kg
Acetone	1.2E-06	lb	1.2E-06	kg
Acid (benzoic)	2.2E-04	lb	2.2E-04	kg
Acid (hexanoic)	4.6E-05	lb	4.6E-05	kg
Acid (unspecified)	8.52	lb	8.52	kg
Alkylated benzenes	4.1E-05	lb	4.1E-05	kg
Alkylated fluorenes	2.4E-06	lb	2.4E-06	kg

Table L-1

DATA FOR THE PRODUCTION
OF POLYETHER POLYOL FOR FLEXIBLE FOAM POLYURETHANES
(Cradle-to-Polyol)
(page 3 of 4)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Alkylated naphthalenes	6.7E-07	lb	6.7E-07	kg
Alkylated phenanthrenes	2.8E-07	lb	2.8E-07	kg
Aluminum	0.020	lb	0.020	kg
Ammonia	0.017	lb	0.017	kg
Antimony	1.3E-05	lb	1.3E-05	kg
Arsenic	4.2E-05	lb	4.2E-05	kg
Barium	0.27	lb	0.27	kg
Benzene	2.4E-04	lb	2.4E-04	kg
Beryllium	2.6E-06	lb	2.6E-06	kg
BOD	0.85	lb	0.85	kg
Boron	6.8E-04	lb	6.8E-04	kg
Bromide	0.027	lb	0.027	kg
Cadmium	6.5E-06	lb	6.5E-06	kg
Calcium	0.45	lb	0.45	kg
Chlorides	5.58	lb	5.58	kg
Chromium (unspecified)	0.0034	lb	0.0034	kg
Cobalt	4.8E-06	lb	4.8E-06	kg
COD	3.45	lb	3.45	kg
Copper	5.9E-05	lb	5.9E-05	kg
Cyanide	8.5E-09	lb	8.5E-09	kg
Dibenzofuran	2.2E-08	lb	2.2E-08	kg
Dibenzothiophene	1.8E-08	lb	1.8E-08	kg
Dissolved Solids	51.3	lb	51.3	kg
Ethylbenzene	2.1E-05	lb	2.1E-05	kg
Fluorides	2.3E-05	lb	2.3E-05	kg
Fluorene	1.1E-06	lb	1.1E-06	kg
Hydrocarbons	0.89	lb	0.89	kg
Iron	0.037	lb	0.037	kg
Lead	1.1E-04	lb	1.1E-04	kg
Lead 210	2.3E-14	lb	2.3E-14	kg
Lithium	0.089	lb	0.089	kg
Magnesium	0.090	lb	0.090	kg
Manganese	1.3E-04	lb	1.3E-04	kg
Mercury	7.9E-07	lb	7.9E-07	kg
Metal Ion (unspecified)	1.00	lb	1.00	kg
Methyl Chloride	4.7E-09	lb	4.7E-09	kg
Methyl Ethyl Ketone	9.5E-09	lb	9.5E-09	kg
Molybdenum	5.0E-06	lb	5.0E-06	kg
Naphthalene	4.0E-06	lb	4.0E-06	kg
n-Decane	6.3E-06	lb	6.3E-06	kg
n-Docosane	1.3E-07	lb	1.3E-07	kg
n-Dodecane	1.2E-05	lb	1.2E-05	kg
n-Eicosane	3.3E-06	lb	3.3E-06	kg
n-Hexacosane	7.9E-08	lb	7.9E-08	kg
n-Hexadecane	1.3E-05	lb	1.3E-05	kg
Nickel	5.1E-05	lb	5.1E-05	kg
Nitrates	1.00	lb	1.00	kg
Nitrogen	0.0025	lb	0.0025	kg
n-Octadecane	3.3E-06	lb	3.3E-06	kg
p -Xylene	2.3E-06	lb	2.3E-06	kg
o -Xylene	2.3E-06	lb	2.3E-06	kg
o-Cresol	6.3E-06	lb	6.3E-06	kg
Oil	0.0097	lb	0.0097	kg

Table L-1

DATA FOR THE PRODUCTION
OF POLYETHER POLYOL FOR FLEXIBLE FOAM POLYURETHANES
(Cradle-to-Polyol)
(page 4 of 4)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
p-Cresol	6.8E-06	lb	6.8E-06	kg
p-Cymene	1.2E-08	lb	1.2E-08	kg
Pentamethylbenzene	8.8E-09	lb	8.8E-09	kg
Phenanthrene	1.7E-07	lb	1.7E-07	kg
Phenol/ Phenolic Compounds	1.14	lb	1.14	kg
Tetradecane	5.1E-06	lb	5.1E-06	kg
Radium 226	7.9E-12	lb	7.9E-12	kg
Radium 228	4.0E-14	lb	4.0E-14	kg
Selenium	2.9E-06	lb	2.9E-06	kg
Silver	2.7E-04	lb	2.7E-04	kg
Sodium	1.29	lb	1.29	kg
Sodium Hydroxide	1.22	lb	1.22	kg
Strontium	0.012	lb	0.012	kg
Styrene	7.5E-07	lb	7.5E-07	kg
Sulfates	0.0093	lb	0.0093	kg
Sulfides	1.0E-04	lb	1.0E-04	kg
Sulfur	5.4E-04	lb	5.4E-04	kg
Surfactants	1.1E-04	lb	1.1E-04	kg
Suspended Solids	2.39	lb	2.39	kg
Thallium	2.7E-06	lb	2.7E-06	kg
Tin	5.0E-05	lb	5.0E-05	kg
Titanium	1.9E-04	lb	1.9E-04	kg
TOC	0.011	lb	0.011	kg
Toluene	2.9E-04	lb	2.9E-04	kg
Total biphenyls	2.7E-06	lb	2.7E-06	kg
Total dibenzothiophenes	8.2E-09	lb	8.2E-09	kg
Vanadium	2.2E-05	lb	2.2E-05	kg
Xylene, unspecified	1.0E-04	lb	1.0E-04	kg
Yttrium	1.5E-06	lb	1.5E-06	kg
Zinc	0.0016	lb	0.0016	kg

References: Tables B-2 through B-6, E-2, F-2, F-4, F-5, I-2, I-3b, K-3, and L-2 through L-7.

Source: Franklin Associates, A Division of ERG models

Table L-2 displays the energy and emissions for harvesting fresh fruit bunches in Malaysia.

Palm Kernels Production

The FFB are delivered to palm oil mills in lorries or trailers. A small portion of the FFB are shipped in sterilizer cages; the majority are placed in sterilizer cages at the mill, where they are then passed through steam. This sterilization deactivates or kills the enzymes, which cause the breakdown of oil into free fatty acids (FFA), which are undesirable in the palm oil. The industry tries to keep the entering FFA to less than 5 percent (Reference L-2). The sterilization process also helps loosen the individual fruit from the bundles.

From the sterilizer, the fruit bunches are sent to a stripper where the fruitlets are separated from then stalk/stem. The empty bunches, approximately 70 percent moisture, are sent to an incinerator (no energy recovery). The resulting incinerator ash, 0.5 percent of the weight of the FFB, is then landspread on the plantation.

The fruitlets from the stripper are sent to a digester where the fruitlets are converted by a mechanical stirring process into homogeneous oily mash. A screw press is used to remove the majority of crude palm oil from the digested mash.

Table L-2

DATA FOR THE GROWING AND HARVESTING OF FRESH FRUIT BUNCHES

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Diesel	1.96	gal	311	16.4	liter	0.72
Total Process			311			0.72
Transportation Energy						
Single unit truck	6.30	ton-miles		20.3	tonne-km	
Diesel	0.14	gal	22.5	1.18	liter	0.052
Total Transportation			22.5			0.052
Environmental Emissions						
Atmospheric Emissions						
Carbon Dioxide (Non-fossil)	8.56	lb		8.56	kg	
Carbon Monoxide	0.0023	lb		0.0023	kg	
Hydrocarbons	0.0010	lb		0.0010	kg	
Nitrogen Oxides	0.0055	lb		0.0055	kg	
Particulates (unknown)	0.066	lb		0.066	kg	
Sulfur Oxides	0.0023	lb		0.0023	kg	
Solid Wastes						
Landfilled	0.012	lb		0.012	kg	

References: L-3 and L-5 through L-9.

Source: Franklin Associates, A Division of ERG

At this point the crude palm oil contains oil, water, and fruit solids. Therefore, the liquid is clarified in a continuous settling tank operation. The decanted palm oil passes through a centrifugal purifier from which the oil layer is vacuum dried to remove any remaining solids and moisture. The oil is then pumped to storage tanks before it is sent on for refining. Crude palm oil yields are approximately 21 percent, by weight, of the FFB.

The deoiled fiber/nut press cake passes to an air separation system, which separates the fiber from the nut. After separation the fiber (30 percent moisture) is used as a fuel for the mill (Reference L-3). The nuts are dried in silo driers and then cracked using centrifugal crackers. The kernel or the nut meat is removed from the shell using air and water separation systems. Kernels are further dried in silo driers and stored awaiting shipment to a processor. Dried kernels account for 6 percent of the FFB weight and contain between 40 and 50 percent oil.

The shells, 15 percent moisture (Reference L-3), are mixed with the fiber and used as boiler fuel. Most boiler designs limit the ratio of fiber/shell feed. For this reason excess shell material typically requires alternative handling. The most common practiced is to use the shell material as a base or surface material on the numerous roads of the plantation (Reference L-3).

Bunch ash, crude palm oil, and shells used in road construction have been treated as coproducts, for which credit has been given on a mass basis. The energy recovered from fiber and shells used as a fuel in this process, as well as any biogas utilization, is greater than the process energy demands. Therefore, only transportation energy is reported for palm oil production. Because the amount of palm kernels produced is relatively small, separate processing plants have been established for extracting palm kernel oil.

The major environmental discharges from a palm oil mill are atmospheric emissions from the incinerator and boiler operations, solid waste in the form of the boiler ash and wastewater treatment sludges, and waterborne wastes in the form of treated palm oil mill effluents (POME) discharged to the water.

The POME has received considerable attention because of the amount of material generated. POME generation is approximately 60 to 67 percent of the weight of FFB, including water form the process. The largest single source of POME is the centrifugal sludge. The quantity of POME on a wet basis is roughly 2.5 times greater than the amount of crude palm oil generated.

Significant research has been performed on the utilization of palm mill wastes including the POME. All raw effluents receive treatment prior to discharge. Data from individual mills as well as government published sources were used in characterizing these discharges. Some general assumptions were necessary to describe the common practices. In general, it was assumed 5 percent of POME is treated through biogas operation; 95 percent is assumed lagooned after aerobic and anaerobic digestion. Of that POME lagooned, 33 percent is utilized as fertilizer, and 65 percent is not utilized; the remaining 2 percent is assumed to have no effluent or zero discharge. The wastewater discharges, therefore, represent this 65 percent value.

The energy requirements and environmental emissions for the production of palm kernels are shown in Table L-3.

Palm Kernel Oil Processing

The extraction of crude palm kernel oil (CPKO) from palm kernels can be carried out in a variety of ways:

- Mechanical extraction using high-pressure screw pressing
- Solvent extraction with hexane
- Preprocessing followed by solvent extraction

Table L-3

DATA FOR THE PRODUCTION OF PALM KERNELS

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Fresh Fruit Bunches	2,980	lb		2,980	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Biomass			3,800			8.85
Total Process			3,800			8.85
Transportation Energy						
Single unit truck	6.22	ton-miles		20.0	tonne-km	
Diesel	0.14	gal	22.2	1.17	liter	0.052
Ocean freighter	1,508	ton-miles		4,854	tonne-km	
Diesel	0.29	gal	46	2.39	liter	0.11
Residual	2.58	gal	443	21.5	liter	1.03
Total Transportation			510			1.19
Environmental Emissions						
Atmospheric Emissions						
Carbon Dioxide (non-fossil)	631	lb		631	kg	
Carbon Monoxide	0.11	lb		0.11	kg	
Methane	23.0	lb		23.0	kg	
Nitrogen Oxides	0.27	lb		0.27	kg	
NM Hydrocarbons	0.52	lb		0.52	kg	
Odorous Sulfur	0.15	lb		0.15	kg	
Particulates (unknown)	3.00	lb		3.00	kg	
Sulfur Oxides	1.05	lb		1.05	kg	
Solid Wastes						
Landfilled	19.7	lb		19.7	kg	
Waterborne Wastes						
BOD	0.18	lb		0.18	kg	
COD	1.63	lb		1.63	kg	
Dissolved Solids	5.07	lb		5.07	kg	
Nitrogen	0.10	lb		0.10	kg	
Oil	0.048	lb		0.048	kg	
Suspended Solids	0.73	lb		0.73	kg	

References: L-3, L-5, L-7, L-8, and L-10 through L-21.

Source: Franklin Associates, A Division of ERG

Industry sources have indicated solvent extraction of palm kernel oil accounts for only a minor portion of the CPKO production. Mechanical extraction may be carried out in either a single-or double-press system. In this analysis it was assumed only one-third of all CPKO is produced by way of a double-press system. The remainder was assumed produced from a single-press system (Reference L-4).

The energy and emissions data for the production of CPKO is presented in Table L-4. For every 1,000 pounds of CPKO produced, 1,560 pounds of cake and pellets are produced. Mass partitioning was used to give credit to these coproducts.

Table L-4

DATA FOR THE PROCESSING OF CRUDE PALM KERNEL OIL

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Palm Kernels	1,064	lb		1,064	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	137	kwh	1,410	302	kwh	3.28
Natural gas	36.1	cu ft	40.4	2.25	cu meters	0.094
Distillate oil	3.83	gal	608	32.0	liter	1.42
Total Process			2,059			4.79
Transportation Energy						
Single unit truck	6.22	ton-miles		20.02	tonne-km	
Diesel	0.14	gal	22.2	1.17	liter	0.052
Ocean freighter	1,508	ton-miles		4,854	tonne-km	
Diesel	0.29	gal	46	2.39	liter	0.11
Residual	2.58	gal	443	21.5	liter	1.03
Total Transportation			510			1.19
Environmental Emissions						
Solid Wastes						
Landfilled	17.2	lb		17.2	kg	
Waterborne Wastes						
Suspended solids	1.84	lb		1.84	kg	

References: L-5, L-7 through L-9, and L-22 through L-24.

Source: Franklin Associates, A Division of ERG

Palm Kernel Oil Refining, Bleaching, and Deodorizing

The purpose for refining is to produce a bland, light colored oil with excellent oxidative stability. This can be achieved by removing trace components such as beta-carotenes, metals, and free fatty acid (FFA). The two most common methods are the alkali or chemical refining route and the physical or steam refining route. The methods differ basically in the way the FFA is removed from the oil.

The chemical refining route is the older of the commercial refining methods. In this system the oil is treated with phosphoric acid and neutralized with a solution of caustic soda. The precipitated impurities are removed and commonly called soapstock. The refined oil is then vacuum dried and mixed with bleaching clay (0.6 to 1.2 percent by weight of the oil input) (Reference L-2). The final step is to deodorize the oil by distillation. The refining loss index for the alkali process ranges from 1.5 to 1.8 times the input FFA.

Drawbacks from the alkali process include the problem of effluent production and the limitation of needing low FFA in the crude oil input. The effluents issue pertains to the production of alkali metal sulphate and dilute sulfuric acid. The alkali method is also considered as restricted to processing crude oils of low FFA. Thus, the greater the incoming FFA, the greater the refinery losses. Typically the FFA levels of crude oils processed by the alkali method are below 0.25 percent (crude palm oil ranges between 3 and 5 percent FFA).

Physical refining, which eliminates the need for effluent plants, involves subjecting the oil to steam distillation of fatty acids in a vacuum under high temperatures. Approximately 85-90 percent of Malaysia refining capacity is through the physical route. Discussion and analysis will therefore focus on physical refining for the processing of crude palm oil.

Physical refining was initially conceived for the treatment of high FFA oils. Because of this situation and the fact that no alkali or acid industry exists in Malaysia, the physical refining route was a natural progression.

Initially the oil is treated with phosphoric acid (85 percent). Next the degummed oil comes in contact with bleaching clay (0.6 to 1.5 percent by weight of the oil) (Reference L-4). This bleaching ratio is considerably higher than that required in the residual/unreacted phosphoric acid and to remove metals and other impurities.

The resulting (degummed and bleached) oil must be deodorized. Because the FFA at this point is still quite high, deodorizing is significantly different than for the alkali process. The deodorization is performed under a vacuum at temperatures of 260° Celsius. The fatty acid distillate is marketed as animal feed. The refining loss index is from 1.1 to 2.8 times the input FFA. An average 93.5 percent oil yield is achieved through the physical refining route.

The energy requirements and environmental emissions for the refining, bleaching, and deodorizing of palm kernel oil are shown in Table L-5.

Table L-5

DATA FOR THE REFINING, BLEACHING AND DEODORIZING OF PALM KERNEL OIL

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Crude Palm Kernel Oil	1,016	lb		1,016	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	4.30	kwh	44.3	9.48	kwh	0.10
Distillate oil	3.20	gal	508	26.7	liter	1.18
Total Process			552			1.29
Transportation Energy						
Combination truck	18.6	ton-miles		59.9	tonne-km	
Diesel	1.18	gal	187	9.85	liter	0.44
Ocean freighter	1,508	ton-miles		4,854	tonne-km	
Diesel	0.45	gal	71.5	3.75	liter	0.17
Residual	4.53	gal	777	37.8	liter	1.81
Total Transportation			1,036			2.41
Environmental Emissions						
Atmospheric Emissions						
Carbon Monoxide	0.0070	lb		0.0070	kg	
Hydrocarbons	0.0020	lb		0.0020	kg	
Solid Wastes						
Landfilled	20.9	lb		20.9	kg	
Waterborne Wastes						
BOD	0.44	lb		0.44	kg	
COD	0.87	lb		0.87	kg	
Suspended solids	0.54	lb		0.54	kg	
Dissolved solids	1.00	lb		1.00	kg	
Oil	0.057	lb		0.057	kg	

References: L-5

Source: Franklin Associates, A Division of ERG

Glycerine Production

Glycerine is produced by several methods: 1) as a byproduct of soap manufacture, 2) from propylene and chlorine to form allyl chloride, which is converted to dichlorohydrin with hypochlorous acid and then saponified to glycerine with caustic, 3) by isomerization of propylene oxide to allyl alcohol, which is then reacted with peracetic acid, followed by hydrolyzing the glycidol into glycerine, 4) hydrogenation of carbohydrates with a nickel catalyst, and 5) from acrolein and hydrogen peroxide. In this analysis, glycerine is produced as a byproduct of palm oil methyl ester, which is an intermediate in soap production. This production method makes up approximately 75 percent of the total U.S. glycerine production amount (Reference L-25).

Although a number of raw materials (coconut oil, palm oil, palm kernel oil, etc.) can be used to produce glycerine, palm kernel oil has been chosen in this analysis (Reference L-26). Refined palm kernel oil is converted to methyl esters and glycerine by the transesterification of triglycerides. The reaction occurs with excess methanol, a process known as methanolysis, in the presence of a sodium methylate catalyst. The reaction takes place at atmospheric pressure and can be carried out in a batch or continuous process. The yields will be higher (in excess of 99 percent) for the continuous process.

The reaction forms two layers. The bottom layer consists of crude glycerine, soap, methanol, small amounts of methyl ester, and water. The top layer contains the methyl esters.

The first step in refining the glycerine is to distill off the methanol and water. The methanol is dried and recirculated back into the esterification process or used to make sodium methylate. The remaining glycerine mixture is acidulated to separate the fatty acids from the soap. Methyl esters are also separated and the glycerine is dried.

Table L-6 displays the energy requirements and environmental emissions for the production of glycerine.

Table L-6

DATA FOR THE PRODUCTION OF GLYCERINE

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Refined Palm Kernel Oil	675	lb		675	kg	
Crude Palm Kernel Oil	232	lb		232	kg	
Methanol	124	lb		124	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	5.48	kwh	56.4	12.1	kwh	0.13
Natural gas	2,071	cu ft	2,320	129	cu meters	5.40
Bit./Sbit. Coal	49.1	lb	551	49.1	kg	1.28
Total Process			2,927			6.81
Transportation Energy						
Combination truck	27.1	ton-miles		87.2	tonne-km	
Diesel	0.28	gal	45.2	2.37	liter	0.11
Rail	49.8	ton-miles		160	tonne-km	
Diesel	0.12	gal	19.6	1.03	liter	0.046
Total Transportation			64.8			0.15
Environmental Emissions						
Atmospheric Emissions						
NM Hydrocarbons	2.41	lb		2.41	kg	
Methane	0.014	lb		0.014	kg	
Other Organics	0.034	lb		0.034	kg	
Waterborne Wastes						
BOD	0.063	lb		0.063	kg	
COD	0.070	lb		0.070	kg	
Oil	0.012	lb		0.012	kg	
Suspended solids	0.028	lb		0.028	kg	
Dissolved solids	0.068	lb		0.068	kg	

References: L-5, L-27, and L-28.

Source: Franklin Associates, A Division of ERG

Polyether Polyol for Flexible Foam Polyurethanes

The manufacture of polyether polyol begins with the introduction of a potassium hydroxide catalyst to a polyol initiator, such as a triol. Sodium hydroxide data is used in place of potassium hydroxide data, which were not available. The manufacture of sodium hydroxide utilizes a process similar to the manufacture of potassium hydroxide. This solution is reacted with propylene oxide and ethylene oxide to form an intermediate. Water is then added to this intermediate. A solvent is introduced, which absorbs the polyol from the water/catalyst. The density difference between the aqueous & organic phases is used to separate the two phases. Finally, the polyol is purified of solvent, side products and water through distillation (Reference L-28).

Table L-7 presents the data for the production of polyether polyol for use in flexible foam polyurethane. Data for the production of polyether polyol were provided by five leading producers (5 plants) in North America to Franklin Associates under contract to Plastics Division of the American Chemistry Council (ACC). Heat was a coproduct for two producers. The energy for exported heat was reported separately as recovered energy.

As of 2002, it is estimated that for all polyurethane applications, there were 7 polyether polyol producers and 9 polyether polyol plants in the U.S. (Reference L-1 and L-29). The polyether polyol data collected represents a majority of the total North American production of polyether polyol for flexible foam polyurethane. The polyether polyol producers who provided data for this module verified that the characteristics of their plants are representative of a majority of the North American production. The average dataset was reviewed and accepted by all polyether polyol data providers.

To assess the quality of the data collected for polyether polyols used in flexible foam polyurethane, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for these polyether polyols include direct measurements, information provided by purchasing and utility records, and engineering estimates. All data submitted for polyether polyols represents the years 2003 and 2005 and represents U.S. production.

Table L-7

DATA FOR THE PRODUCTION OF POLYETHER POLYOL FOR FLEXIBLE FOAM POLYURETHANE

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Propylene oxide	856	lb			856	kg	
Ethylene oxide	113	lb			113	kg	
Glycerine	26.3	lb			26.3	kg	
Caustic Potash	3.96	lb			3.96	kg	
Water Consumption	54.0	gal			451	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	10.9	kwh		112	24.0	kwh	0.26
Electricity (cogeneration)	322	cu ft	(1)	361	20.1	cu meters	0.84
Natural gas	985	cu ft		1,103	61.5	cu meters	2.57
Recovered Energy	79.0	thousand Btu		79.0	184	MJ	0.18
Total Process				1,497			3.49
Environmental Emissions							
Atmospheric Emissions							
Carbon Monoxide	0.027	lb			0.027	kg	
Carbon Dioxide	26.1	lb			26.1	kg	
Chlorine	1.0E-05	lb	(2)		1.0.E-05	kg	
Lead	1.0E-07	lb	(2)		1.0.E-07	kg	
Mercury	1.0E-07	lb	(2)		1.0.E-07	kg	
Methane	0.0010	lb	(2)		0.0010	kg	
Nitrogen Oxides	0.063	lb			0.063	kg	
Nitrous Oxide	1.0E-04	lb	(2)		1.0E-04	kg	
NM Hydrocarbons	0.11	lb			0.11	kg	
Other Organics	0.023	lb			0.023	kg	
Particulates (unknown)	0.0010	lb	(2)		0.0010	kg	
PM2.5	0.010	lb	(2)		0.010	kg	
PM10	0.057	lb			0.057	kg	
Sulfur Oxides	2.1E-04	lb			2.1E-04	kg	
Solid Wastes							
Landfilled	0.87	lb			0.87	kg	
Waterborne Wastes (3)							
Ammonia	0.010	lb	(2)		0.010	kg	
BOD	0.28	lb			0.28	kg	
COD	2.96	lb			2.96	kg	
Dissolved Solids	1.00	lb	(2)		1.00	kg	
Hydrocarbons	0.10	lb	(2)		0.10	kg	
Metal Ion	1.00	lb	(2)		1.00	kg	
Nitrates	1.00	lb	(2)		1.00	kg	
Suspended Solids	3.6.E-04	lb			3.6E-04	kg	
TOC	0.010	lb	(2)		0.010	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(3) These waterborne emissions may be overstated as 1 or more of the plants providing data were only able to supply waterborne emissions before the effluent was sent to a water treatment plant.

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Source: Franklin Associates, A Division of ERG

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L-29. Research by Franklin Associates on each polyol producing companies' website.

APPENDIX M

METHYLENE DIPHENYLENE DIISOCYANATE (MDI)

INTRODUCTION

This appendix discusses the manufacture of pure and polymeric forms of methylene diphenylene diisocyanate (MDI), which is a precursor for a variety of polyurethanes. Industries that use polyurethanes with MDI as a precursor include automotive, construction, footwear, and appliances. Over 2.2 billion pounds of pure and polymeric MDI were produced in the U.S. and Canada in 2002 (Reference M-1). The material flow for MDI is shown in Figure M-1. The total unit process energy and emissions data (cradle-to-MDI) for MDI are displayed in Table M-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following processes are included in this appendix:

- Hydrogen
- Nitric Acid
- Nitrobenzene
- Aniline
- Formaldehyde
- Phosgene
- Methylene diphenylene diisocyanate (PMDI/MDI)

Crude oil production, refining of petroleum products (distillation, desalting and hydrotreating), natural gas production, and natural gas processing (extraction) are discussed in Appendix B. Carbon monoxide production, and methanol production are discussed in Appendix F. Benzene production and pygas production are discussed in Appendix G. Salt mining and sodium hydroxide/chlorine production are discussed in Appendix I. Ammonia production is discussed in Appendix J. Although carbon monoxide data is not shown in this appendix due to confidentiality issues, the transport data is specific to MDI and is represented as 0.0324 ton-miles by natural gas pipeline in Table M-4.

Hydrogen Production

Hydrogen and carbon dioxide are coproducts in the production of syntheses gas. Synthesis gas is primarily produced from natural gas by steam-methane reforming. Natural gases, or other light hydrocarbons, and steam are fed into a primary reformer over a nickel catalyst to produce hydrogen and carbon oxides, generally referred to as synthesis gas. About 70 percent of the hydrocarbon feed is converted to synthesis gas in the primary reformer.

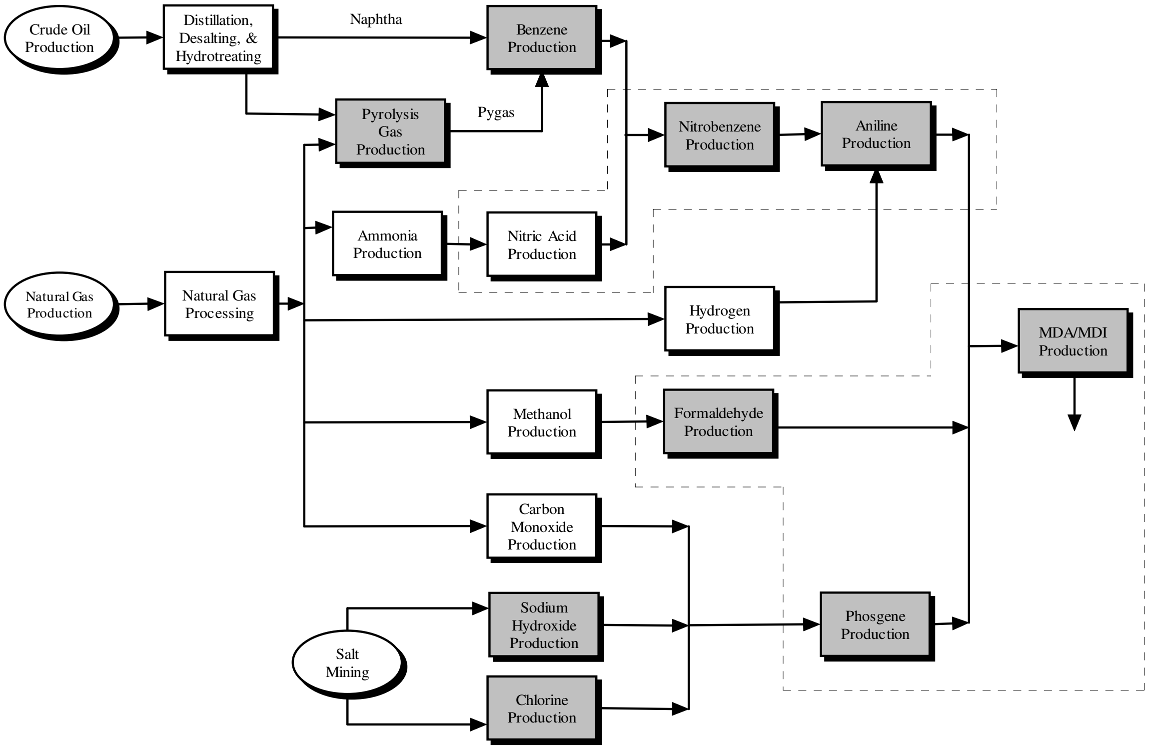

Figure M-1. Flow diagram for the manufacture of methylene diphenylene diisocyanate (MDI). Shaded boxes represent partial or complete data provided by manufacturers specifically for this analysis. Boxes within the dotted lines are included in an aggregated dataset.

The effluent from the reformers is fed into carbon monoxide shift converters where the carbon monoxide reacts with water to form carbon dioxide and hydrogen. The effluent from the shift converters is cooled, and condensed water is removed. The carbon dioxide and some excess hydrogen are also removed from the synthesis gas as coproducts (Reference M-2).

The ratio of carbon monoxide to hydrogen in the synthesis gas differs depending on the specifications for the synthesis gas, and therefore the amounts of hydrogen and carbon dioxide coproducts differ also. Synthesis gas is a raw material for many different processes, each with specific requirements. Because of this difference in requirements, it is difficult to show a generic or widely applicable material balance for this process.

Table M-1

DATA FOR THE PRODUCTION OF METHYLENE DIPHENYLENE DIISOCYANATE (MDI)
(Cradle-to-MDI)
(page 1 of 4)

	English units (Basis: 1,000 lb)			Per 1,000 kg		
Raw Materials						
Crude oil	335	lb		335	kg	
Natural Gas	363	lb		363	kg	
Salt	386	lb		386	kg	
Oxygen from air	360	lb		360	kg	
Water	257	gal		2,144	liter	
Nitrogen from air	40.7	lb		40.7	kg	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Energy of Material Resource						
Natural Gas			7,766			18.1
Petroleum			6,280			14.6
Total Resource			14,046			32.7
Process Energy						
Electricity (grid)	293	kwh	3,112	645	kwh	7.25
Electricity (cogeneration)	843	cu ft (2)	867	53	cu meters	2.02
Natural gas	5,411	cu ft	6,060	338	cu meters	14.1
LPG	0.048	gal	5.23	0.40	liter	0.012
Bit./Sbit. Coal	15.4	lb	173	15.4	kg	0.40
Distillate oil	0.74	gal	118	6.19	liter	0.27
Residual oil	2.84	gal	487	23.7	liter	1.13
Gasoline	0.063	gal	8.95	0.53	liter	0.021
Diesel	2.6E-04	gal	0.042	2.2E-03	liter	9.7E-05
Internal Offgas use (1)						
From Oil	16.8	lb	453	16.8	kg	1.05
From Natural Gas	23.2	lb	626	23.2	kg	1.46
Recovered Energy	956	th Btu	956	2,224	MJ	2.23
Total Process			10,955			25.5
Transportation Energy						
Combination truck	6.62	ton-miles		21.3	tonne-km	
Diesel	0.069	gal	11.0	0.58	liter	0.026
Rail	33.3	ton-miles		107	tonne-km	
Diesel	0.083	gal	13.1	0.69	liter	0.030
Barge	59.4	ton-miles		191	tonne-km	
Diesel	0.048	gal	7.54	0.40	liter	0.018
Residual oil	0.16	gal	27.1	1.32	liter	0.063
Ocean freighter	518	ton-miles		1,666	tonne-km	
Diesel	0.10	gal	15.6	0.82	liter	0.036
Residual	0.89	gal	152	7.39	liter	0.35
Pipeline-natural gas	192	ton-miles		618	tonne-km	
Natural gas	133	cu ft	149	8.27	cu meter	0.35
Pipeline-petroleum products	151	ton-miles		485	tonne-km	
Electricity	3.29	kwh	33.7	7.25	kwh	0.078
Total Transportation			408			0.95

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

(2) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency. If offgas was used within the cogen plant, the energy amount is shown within the Internal Offgas use.

Table M-1

DATA FOR THE PRODUCTION
OF METHYLENE DIPHENYLENE DIISOCYANATE (MDI)
(Cradle-to-MDI)
(page 2 of 4)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Aldehydes (unspecified)	2.3E-04	lb	2.3E-04	kg
Ammonia	0.27	lb	0.27	kg
Antimony	7.0E-07	lb	7.0E-07	kg
Arsenic	8.9E-08	lb	8.9E-08	kg
Benzene	0.037	lb	0.037	kg
Carbon Dioxide - Fossil	363	lb	363	kg
Carbon Monoxide	2.11	lb	2.11	kg
Carbon Tetrachloride	8.9E-05	lb	8.9E-05	kg
CFC 13 (Methane, trichlorofluoro-)	7.5E-06	lb	7.5E-06	kg
Chlorine	6.8E-04	lb	6.8E-04	kg
Chromium	2.3E-07	lb	2.3E-07	kg
Copper	4.8E-05	lb	4.8E-05	kg
Dimethyl Ether	0.0010	lb	0.0010	kg
Ethylbenzene	0.0044	lb	0.0044	kg
Ethylene Dibromide	1.5E-06	lb	1.5E-06	kg
HCFC-123	3.7E-05	lb	3.7E-05	kg
HCFC-22	4.8E-04	lb	4.8E-04	kg
HFC-134a	3.7E-05	lb	3.7E-05	kg
Hydrogen	7.5E-04	lb	7.5E-04	kg
Hydrogen Chloride	2.8E-04	lb	2.8E-04	kg
NMVOC, non-methane volatile organic compounds, unspecified	0.23	lb	0.23	kg
Lead	4.8E-06	lb	4.8E-06	kg
Mercury	7.0E-05	lb	7.0E-05	kg
Methane	3.91	lb	3.91	kg
Methanol	0.0010	lb	0.0010	kg
Nickel	2.0E-06	lb	2.0E-06	kg
Nickel Compounds	4.8E-04	lb	4.8E-04	kg
Nitrogen Oxides	0.58	lb	0.58	kg
Non-Methane Hydrocarbons	0.56	lb	0.56	kg
Other Organics	0.21	lb	0.21	kg
Particulates (PM10)	0.069	lb	0.069	kg
Particulates (PM2.5)	0.018	lb	0.018	kg
Particulates (unspecified)	0.011	lb	0.011	kg
PFCs	0.0048	lb	0.0048	kg
Polyaromatic Hydrocarbons (total)	1.9E-05	lb	1.9E-05	kg
Sulfur Dioxide	0.81	lb	0.81	kg
Sulfur Oxides	0.18	lb	0.18	kg
Sulfuric Acid	4.8E-06	lb	4.8E-06	kg
TOC	0.74	lb	0.74	kg
Toluene	0.057	lb	0.057	kg
VOC	0.30	lb	0.30	kg
Xylene	0.033	lb	0.033	kg
Solid Wastes				
Landfilled	23.4	lb	23.4	kg
Burned	3.26	lb	3.26	kg
Waste-to-Energy	0.75	lb	0.75	kg
Waterborne Wastes				
m-Xylene	5.1E-06	lb	5.1E-06	kg
1-Methylfluorene	9.5E-09	lb	9.5E-09	kg
2,4-Dimethylphenol	4.9E-06	lb	4.9E-06	kg
2-Hexanone	1.2E-06	lb	1.2E-06	kg
2-Methylnaphthalene	2.7E-06	lb	2.7E-06	kg
4-Methyl-2-Pentanone	3.5E-07	lb	3.5E-07	kg
Acetone	8.4E-07	lb	8.4E-07	kg
Acid (benzoic)	1.8E-04	lb	1.8E-04	kg
Acid (hexanoic)	3.7E-05	lb	3.7E-05	kg
Alkylated benzenes	3.3E-05	lb	3.3E-05	kg
Alkylated fluorenes	1.9E-06	lb	1.9E-06	kg
Alkylated naphthalenes	5.5E-07	lb	5.5E-07	kg
Alkylated phenanthrenes	2.3E-07	lb	2.3E-07	kg
Aluminum	0.016	lb	0.016	kg
Ammonia	0.029	lb	0.029	kg

Table M-1

DATA FOR THE PRODUCTION
OF METHYLENE DIPHENYLENE DIISOCYANATE (MDI)
(Cradle-to-MDI)
(page 3 of 4)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Antimony	1.0E-05	lb	1.0E-05	kg
Arsenic	3.4E-05	lb	3.4E-05	kg
Barium	0.22	lb	0.22	kg
Benzene	1.9E-04	lb	1.9E-04	kg
Beryllium	2.2E-06	lb	2.2E-06	kg
BOD	0.34	lb	0.34	kg
Boron	5.5E-04	lb	5.5E-04	kg
Bromide	0.023	lb	0.023	kg
Cadmium	5.3E-06	lb	5.3E-06	kg
Calcium	0.37	lb	0.37	kg
Chlorides	4.57	lb	4.57	kg
Chloroform	1.0E-06	lb	1.0E-06	kg
Chromium (unspecified)	4.4E-04	lb	4.4E-04	kg
Cobalt	3.9E-06	lb	3.9E-06	kg
COD	0.58	lb	0.58	kg
Copper	4.9E-05	lb	4.9E-05	kg
Cyanide	1.0E-06	lb	1.0E-06	kg
Dibenzofuran	1.6E-08	lb	1.6E-08	kg
Dibenzothiophene	1.3E-08	lb	1.3E-08	kg
Dissolved Solids	32.6	lb	32.6	kg
Ethylbenzene	1.2E-05	lb	1.2E-05	kg
Fluorene	9.0E-07	lb	9.0E-07	kg
Iron	0.030	lb	0.030	kg
Lead	9.1E-05	lb	9.1E-05	kg
Lead 210	1.8E-14	lb	1.8E-14	kg
Lithium	0.058	lb	0.058	kg
Magnesium	0.074	lb	0.074	kg
Manganese	1.1E-04	lb	1.1E-04	kg
Mercury	4.2E-07	lb	4.2E-07	kg
Methyl Chloride	3.4E-09	lb	3.4E-09	kg
Methyl Ethyl Ketone	6.7E-09	lb	6.7E-09	kg
Molybdenum	4.0E-06	lb	4.0E-06	kg
Naphthalene	3.2E-06	lb	3.2E-06	kg
n-Decane	5.1E-06	lb	5.1E-06	kg
n-Docosane	9.0E-08	lb	9.0E-08	kg
n-Dodecane	9.7E-06	lb	9.7E-06	kg
n-Eicosane	2.7E-06	lb	2.7E-06	kg
n-Hexacosane	5.6E-08	lb	5.6E-08	kg
n-Hexadecane	1.1E-05	lb	1.1E-05	kg
Nickel	5.2E-05	lb	5.2E-05	kg
Nitrates	1.0E-08	lb	1.0E-08	kg
n-Octadecane	2.6E-06	lb	2.6E-06	kg
p -Xylene	1.9E-06	lb	1.9E-06	kg
o -Xylene	1.9E-06	lb	1.9E-06	kg
o-Cresol	5.1E-06	lb	5.1E-06	kg
Oil	0.029	lb	0.029	kg
p-Cresol	5.5E-06	lb	5.5E-06	kg

Table M-1

DATA FOR THE PRODUCTION
OF METHYLENE DIPHENYLENE DIISOCYANATE (MDI)
(Cradle-to-MDI)
(page 4 of 4)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
p-Cymene	8.4E-09	lb	8.4E-09	kg
Pentamethylbenzene	6.3E-09	lb	6.3E-09	kg
Phenanthrene	1.4E-07	lb	1.4E-07	kg
Phenol/ Phenolic Compounds	3.7E-04	lb	3.7E-04	kg
Phosphates	0.0071	lb	0.0071	kg
Tetradecane	4.1E-06	lb	4.1E-06	kg
Radium 226	6.4E-12	lb	6.4E-12	kg
Radium 228	3.3E-14	lb	3.3E-14	kg
Selenium	2.5E-06	lb	2.5E-06	kg
Silver	2.3E-04	lb	2.3E-04	kg
Sodium	1.07	lb	1.07	kg
Strontium	0.0096	lb	0.0096	kg
Styrene	1.4E-07	lb	1.4E-07	kg
Sulfates	0.0077	lb	0.0077	kg
Sulfides	4.9E-04	lb	4.9E-04	kg
Sulfur	4.4E-04	lb	4.4E-04	kg
Surfactants	9.0E-05	lb	9.0E-05	kg
Suspended Solids	1.87	lb	1.87	kg
Thallium	2.2E-06	lb	2.2E-06	kg
Tin	4.1E-05	lb	4.1E-05	kg
Titanium	1.6E-04	lb	1.6E-04	kg
TOC	0.025	lb	0.025	kg
Toluene	1.9E-04	lb	1.9E-04	kg
Total biphenyls	2.2E-06	lb	2.2E-06	kg
Total dibenzothiophenes	6.7E-09	lb	6.7E-09	kg
Vanadium	2.3E-05	lb	2.3E-05	kg
Xylene, unspecified	8.4E-05	lb	8.4E-05	kg
Yttrium	1.2E-06	lb	1.2E-06	kg
Zinc	3.7E-04	lb	3.7E-04	kg

References: Tables B-2 through B-5, F-2, G-2, G-3, I-2, I-3b, J-2, and M-2 through M-4.

Source: Franklin Associates, A Division of ERG models

Table M-2 provides the energy and emissions data for the production of hydrogen. The data for hydrogen production are estimates of the synthesis gas production. Raw material inputs for hydrogen are based on the conversion of methane to carbon monoxide and hydrogen.

Nitric Acid Production

The raw materials necessary for nitric acid production are ammonia, air, and a platinum-rhodium catalyst. Gaseous ammonia is mixed with air and passed over the catalyst to produce nitric oxides. Reaction water is removed as 2% nitric acid condensate. Secondary air containing recycled nitrogen dioxide is added to the nitrous gas, which is compressed and fed into an absorption column, where acid is formed. Nitrogen dioxide remaining in the gas is absorbed in the nitric acid and must be stripped from the acid by secondary air, which is recycled.

The energy and emissions data for nitric acid production is from a primary European source from 1990. This dataset has been included with the aniline/ nitrobenzene average dataset in Table M-3 to conceal the confidential data of the provider company.

Table M-2

DATA FOR THE PRODUCTION OF HYDROGEN
VIA NATURAL GAS STEAM REFORMING AND SHIFT REACTION

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Material Inputs						
Processed Natural Gas	2,908	lb		2,908	kg	
Water	576	gal		4,804	liter	
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	143	kwh	1,525	316	kwh	3.55
Natural gas	1,126	cu ft	1,261	70.3	cu meters	2.93
Total Process			2,785			6.48
Transportation Energy						
Pipeline-natural gas	1.20	ton-miles		3.86	tonne-km	
Natural gas	0.83	cu ft	0.93	2.66	cu meters	2.98
Total Transportation			0.93			2.98
Environmental Emissions						
Atmospheric Emissions						
Total Organic Compounds	3.60	lb		3.60	kg	
Carbon Monoxide	6.90	lb		6.90	kg	
Sulfur oxides	0.029	lb		0.029	kg	
Carbon Dioxide (fossil)	7,996	lb		7,996	kg	

References: M-2, M-3, M-4, M-11, and M-12.

Source: Franklin Associates, A Division of ERG

Nitrobenzene Production

Nitrobenzene and other nitroaromatics, such as nitrochlorobenzene and dinitrotoluene, are formed by nitrating the appropriate aromatic hydrocarbon with a mixed acid containing nitric and sulfuric acid. The nitrated aromatic is separated from the acid mixture in a centrifugal separator, neutralized and washed, and finally dried in a drying column. The recovered acid mixture containing nitric acid and nitro compounds is recycled.

The energy and emissions data for nitrobenzene production are from two provider companies and are aggregated with the aniline/nitric acid dataset in Table M-3 to protect the data's confidentiality.

As of 2002 there were 4 nitrobenzene producers and 5 nitrobenzene plants in the U.S. (Reference M-6). The nitrobenzene data collected represents a majority of the total North American nitrobenzene production amount. The nitrobenzene producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American nitrobenzene production. The average dataset was reviewed and accepted by all nitrobenzene data providers.

To assess the quality of the data collected for nitrobenzene, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for nitrobenzene include direct measurements, information provided by purchasing and utility records and engineering estimates. All data submitted for nitrobenzene ranges from 2003-2004 and represents U.S. production.

Aniline Production

Aniline is formed by the hydrogenation of nitrobenzene in the presence of a copper-chromium or copper-silica catalyst, or by vapor phase ammonolysis of phenol and ammonia.

For hydrogenation of nitrobenzene, preheated hydrogen and nitrobenzene are fed into an evaporator, and aniline is formed by vapor phase catalytic reduction. The aniline is dehydrated to remove the water produced during the reaction.

In the ammonolysis process, phenol and ammonia are preheated and fed into an adiabatic, fixed abed reactor and passed over a catalyst to produce aniline and water. The effluent gas is partially condensed, and the liquid and vapor phases separated. The vapor phase containing unreacted ammonia is recycled. Ammonia is stripped from the liquid fraction, and the aniline is dried and distilled. Unreacted phenol is recovered and recycled.

Table M-3 presents the data for the production of nitric acid, nitrobenzene, and aniline. Data for the production of nitrobenzene and aniline were provided by two leading producers (2 plants) in North America to Franklin Associates. Steam/heat is produced as a coproduct during this process. The energy amount for this coproduct is reported separately as recovered energy.

Table M-3

DATA FOR THE PRODUCTION OF ANILINE
(including nitric acid and nitrobenzene production)

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Benzene	848	lb			848	kg	
Hydrogen	63.0	lb			63.0	kg	
Ammonia	203	lb			203	kg	
Oxygen (from air)	559	lb			559	kg	
Water Consumption	141	gal			1,177	liter	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	75.4	kwh		776	166	kwh	1.81
Electricity (cogeneration)	239	cu ft	(1)	268	14.9	cu meters	0.62
Natural gas	451	cu ft		505	28.2	cu meters	1.18
Recovered Energy	1,308	thousand Btu		1,308	3,045	MJ	3.05
Total Process				241			0.56
Transportation Energy							
Barge	14.8	ton-miles			47.6	tonne-km	
Diesel	0.012	gal		1.88	0.099	liter	0.0044
Residual oil	0.039	gal		6.76	0.33	liter	0.016
Pipeline-petroleum products	0.15	ton-miles			0.48	tonne-km	
Electricity	0.0033	kwh		0.033	0.0072	kwh	7.8E-05
Total Transportation				8.67			0.020
Environmental Emissions							
Atmospheric Emissions							
Sulfuric Acid	1.0E-05	lb	(2)		1.0E-05	kg	
Ammonia	0.0033	lb			0.0033	kg	
Carbon Monoxide	0.011	lb			0.011	kg	
Chlorine	9.7E-05	lb			9.7E-05	kg	
Copper	1.0E-04	lb	(2)		1.0E-04	kg	
HCFC-22	0.010	lb	(2)		0.010	kg	
Hydrogen Chloride	1.0E-04	lb	(2)		1.0E-04	kg	
Lead	1.0E-05	lb	(2)		1.0E-05	kg	
Nickel Compounds	0.0010	lb	(2)		0.0010	kg	
Metal Ion	0.0010	lb	(2)		0.0010	kg	
Nitrogen Oxides	0.84	lb			0.84	kg	
NM Hydrocarbons	0.0072	lb			0.0072	kg	
Other Organics	0.010	lb	(2)		0.010	kg	
PFC's	0.010	lb	(2)		0.010	kg	
PM2.5	0.010	lb	(2)		0.010	kg	
PM10	0.045	lb			0.045	kg	
Sulfur Oxides	1.0E-05	lb	(2)		1.0E-05	kg	
Solid Wastes							
Burned	0.50	lb			0.50	kg	
Waste-to-Energy	1.56	lb			1.56	kg	
Waterborne Wastes (3)							
Total Organic Carbon	0.010	lb	(2)		0.010	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(3) Waterborne emissions collected for nitrobenzene and aniline included those sent to deepwell disposal. Emissions sent to deepwell disposal are not included in the table as they are not released to a water source. The following emissions were reported as being sent to deepwell disposal: toluene, phenol, 2-DNP, aniline, and nitrobenzene.

References: M-5 and M-7

Source: Franklin Associates, A Division of ERG

As of 2002 there were 6 aniline producers and 7 aniline plants in the U.S. (Reference M-6). The aniline data collected represents approximately half of the total North American aniline production amount. The aniline producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American aniline production. The average dataset was reviewed and accepted by all aniline data providers.

To assess the quality of the data collected for aniline, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for aniline include direct measurements, information provided by purchasing and utility records, and engineering estimates. All data submitted for aniline ranges from 2003-2004 and represents U.S. production.

Formaldehyde Production

Formaldehyde is most commonly produced by oxidation of methanol, in the presence of either a silver or ferric molybdate catalyst. Along with the silver catalyst, methanol, air, and water are preheated and fed into the reactor vessel. The heat from the reaction gas is recovered by generating steam, and the gases are then sent to an absorption tower.

The process for the metal oxide catalyst differs from the silver catalyst process in that the metal oxide reaction occurs at lower temperatures and requires a much greater excess of air in the feed. Heat recovered from the reaction gases is used to preheat the feed, and the excess steam is exported.

The formaldehyde is stripped from the reaction gases with water and then distilled. A solution containing 60 percent urea can also be used during the stripping process.

Data for the production of formaldehyde was collected from one confidential source in the United States. This data was aggregated with phosgene, MDA, and PMDI/MDI and is included in Table M-4.

As of 2001 there were 16 formaldehyde producers and 43 formaldehyde plants in the U.S. (Reference M-6). Although the formaldehyde data collected represents only a small portion of the total North American formaldehyde production amount, the formaldehyde producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American formaldehyde production.

To assess the quality of the data collected for formaldehyde, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for formaldehyde include direct measurements, information provided by purchasing and utility records, and engineering estimates. All data submitted for formaldehyde represents 2007 U.S. production.

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. 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 was collected with the formaldehyde, MDA and PMDI/MDI energy and emissions and is included in Table M-4.

Methylene Diphenylene Diisocyanate (PMDI/MDI) Production

Methylene diphenylene isocyanate (MDI) formation consists of two steps. In the first, 4,4-methylenedianiline (MDA) is created as an intermediate by the condensation of aniline and formaldehyde in the presence of an acid. In the final step, MDA is phosgenated to produce MDI. A mixture of MDI, its dimer and trimer is formed, and referred to as polymeric MDI (PMDI). Pure MDI is distilled from the reaction mixture. The market split is approximately 80 percent polymeric MDI and 20 percent pure MDI (Reference M-6). Polyurethanes commonly utilize the PMDI for rigid foams, while the pure MDI is more commonly used in thermoplastic and cast elastomer applications (Reference M-8).

Table M-4 presents the data for the production of formaldehyde, phosgene, MDA, and PMDI/MDI. Data for the production of phosgene, MDA, PMDI/MDI were provided by four leading producers (4 plants) in North America to Franklin Associates. Within this process, an offgas is produced from the raw materials entering. A portion of this offgas is used within the process to produce steam. This portion is shown in Table M-4 as "Recovered Energy." A large amount of hydrogen chloride is produced as a coproduct during this process. A mass basis was used to partition the credit for each product. The coproduct amount is not shown due to confidentiality issues. 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. Confidentiality issues prohibit the revealing of each plant's individual HCl coproduct amount. An average of the coproduct could be provided, but this would not allow for precise reproduction of the dataset.

As of 2003 there were 4 PMDI/MDI producers and 5 PMDI/MDI plants in the U.S. (Reference M-6). The PMDI/MDI data collected represents a majority of the total North American PMDI/MDI production amount. The PMDI/MDI producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American PMDI/MDI production. The average dataset was reviewed and accepted by all PMDI/MDI data providers.

To assess the quality of the data collected for PMDI/MDI, the collection methods, technology, industry representation, time period, and geography were considered. The data collection methods for PMDI/MDI include direct measurements, information provided by purchasing and utility records, and engineering estimates. All data submitted for PMDI/MDI represents the year 2003 and represents U.S. production.

Table M-4

DATA FOR THE PRODUCTION OF PURE AND POLYMERIC METHYLENE DIPHENYLENE DIISOCYANATE (MDI)

(including formaldehyde, phosgene and MDA production)

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Aniline	480	lb			480	kg	
Methanol	104	lb			104.1	kg	
Chlorine	378	lb			378	kg	
Caustic	58.2	lb			58.2	kg	
Carbon Monoxide	150	lb			150	kg	
Oxygen from air	52.0	lb			52.0	kg	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	51.8	kwh		533	114	kwh	1.24
Electricity (cogeneration)	246	cu ft	(1)	275	15.3	cu meters	0.64
Natural gas	1,856	cu ft		2,079	116	cu meters	4.84
Recovered Energy	328	thousand Btu		328	763	MJ	0.76
Total Process				2,559			5.96
Transportation Energy							
Combination truck	0.40	ton-miles			1.30	tonne-km	
Diesel	0.0042	gal		0.67	0.035	liter	0.0016
Rail	3.25	ton-miles			10.5	tonne-km	
Diesel	0.0081	gal		1.28	0.067	liter	0.0030
Pipeline-petroleum products	0.045	ton-miles			0.15	tonne-km	
Electricity	9.9E-04	kwh		0.010	0.0022	kwh	2.3E-05
Total Transportation				1.97			0.0046
Environmental Emissions							
Atmospheric Emissions							
Aldehydes	2.3E-04	lb			2.3E-04	kg	
Ammonia	0.0024	lb			0.0024	kg	
Carbon Dioxide	10.0	lb	(2)		10.0	kg	
Carbon Monoxide	0.60	lb			0.60	kg	
Carbon Tetrachloride	1.0E-05	lb			1.0E-05	kg	
Chlorine	1.0E-04	lb			1.0E-04	kg	
Dimethyl ether	0.0010	lb	(2)		0.0010	kg	
Hydrochloric Acid	1.0E-04	lb	(2)		1.0E-04	kg	
Methanol	0.0010	lb	(2)		0.0010	kg	
NM Hydrocarbons	0.014	lb			0.014	kg	
Nitrogen Oxides	0.0010	lb	(2)		0.0010	kg	
Other Organics	0.11	lb			0.11	kg	
Particulates (unknown)	0.0010	lb	(2)		0.0010	kg	
PM2.5	0.0010	lb	(2)		0.0010	kg	
PM10	0.014	lb			0.014	kg	
Sulfur Oxides	1.0E-06	lb	(2)		1.0E-06	kg	
Solid Wastes							
Landfilled	1.38	lb			1.38	kg	
Burned	1.45	lb			1.45	kg	
Waterborne Wastes (3)							
Ammonia	0.0011	lb			0.0011	kg	
BOD	0.0045	lb			0.0045	kg	
Chloroform	1.0E-06	lb	(2)		1.0E-06	kg	
COD	0.010	lb	(2)		0.010	kg	
Copper	1.0E-06	lb	(2)		1.0E-06	kg	
Cyanide	1.0E-06	lb	(2)		1.0E-06	kg	
Dissolved Solids	10.0	lb	(2)		10.0	kg	
Lead	1.0E-07	lb	(2)		1.0E-07	kg	
Nickel	1.0E-05	lb	(2)		1.0E-05	kg	
Nitrates	1.0E-08	lb	(2)		1.0E-08	kg	
Oil	0.010	lb	(2)		0.010	kg	
Phenol	1.0E-04	lb	(2)		1.0E-04	kg	
Phosphates	0.0071	lb			0.0071	kg	
Suspended Solids	0.0083	lb			0.0083	kg	
TOC	0.020	lb			0.020	kg	

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(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

(3) Waterborne emissions collected for phosgene/MDA/MDI included those sent to deepwell disposal. Emissions sent to deepwell disposal are not included in the table as they are not released to a readily accessible aquifer. The following emissions were reported as being sent to deepwell disposal: MDA, aniline, and caustic.

References: M-7 and M-9

Source: Franklin Associates, A Division of ERG

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APPENDIX N

TOLUENE DIISOCYANATE (TDI)

INTRODUCTION

This appendix discusses the manufacture of toluene diisocyanate (TDI), which is a precursor for a variety of polyurethanes, mostly flexible foams. Examples of uses of polyurethanes that have TDI as a precursor are furniture, automotive, and carpet underlayment. Over 1.1 billion pounds of TDI were produced in the U.S. and Canada in 2002 (Reference N-1). The material flow for TDI is shown in Figure N-1. The total unit process energy and emissions data (cradle-to-TDI) for TDI are displayed in Table N-1. Individual process tables on the bases of 1,000 pounds and 1,000 kilograms are also shown within this appendix. Processes that have been discussed in previous appendices have been omitted from this appendix. The following processes are included in this appendix:

- Toluene
- Sulfur
- Sulfuric Acid
- Soda Ash
- Dinitrotoluene
- Toluene diamine (TDA)
- Toluene diisocyanate (TDI)

Crude oil production, refining of petroleum products (distillation, desalting, and hydrotreating), natural gas production, and natural gas processing (extraction) are discussed in Appendix B. Carbon monoxide production is discussed in Appendix F. Salt mining and sodium hydroxide/chlorine production are discussed in Appendix I. Ammonia production is discussed in Appendix J. Nitric acid production and phosgene production are discussed in Appendix M. Although carbon monoxide data is not shown in this appendix due to confidentiality issues, the transport data is specific to TDI and is represented as 0.560 ton-miles by natural gas pipeline in Table N-6.

Toluene Production

Approximately 95 percent of toluene is produced by the catalytic reforming of light petroleum distillate (naphtha). The remainder is produced either from pyrolysis gas or as a coproduct of styrene from ethylbenzene (Reference N-2). Data for toluene in this analysis represents only the reforming process.

In the reforming process, naphtha is fed through a catalyst bed at elevated temperatures and pressures. The most common type of reforming process is platforming, in which a platinum-containing catalyst is used. Products obtained from the platforming process include aromatic compounds (benzene, toluene, xylene), chemical hydrogen, light gas, and liquefied petroleum gas. The aromatics content of the reformate varies and is normally less than 45 percent.

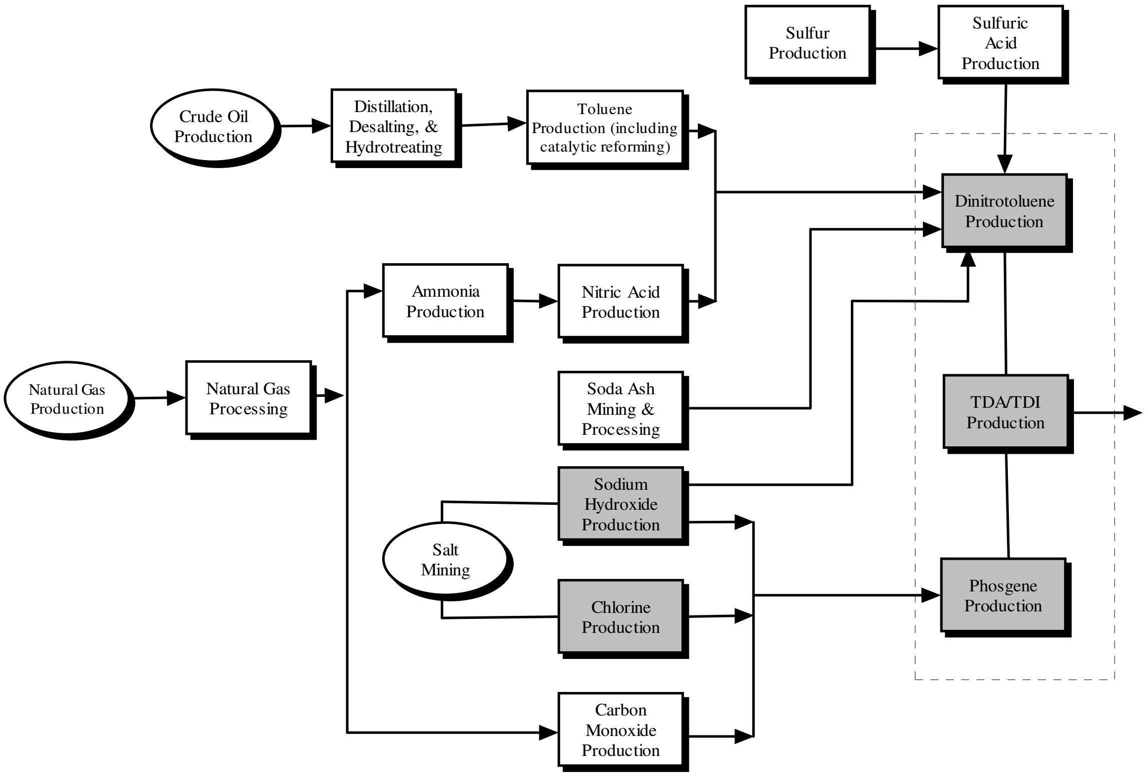

Figure N-1. Flow diagram for the manufacture of toluene diisocyanate (TDI). Shaded boxes represent partial or complete data provided by manufacturers specifically for this analysis. Boxes within the dotted rectangle are included in an aggregate dataset.

The reformate from the platforming 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 N-2. These data are calculated from a straight average of two catalytic reformer datasets from Europe in the early 1990s.

Sulfur Production

Sulfur exists in nature as elemental sulfur and is also found in ores such as pyrite (FeS2). Sulfur is also recovered from hydrogen sulfide (H2S), a component of petroleum and natural gas. The Frasch process (sulfur obtained from limestone) is no longer used in the United States (Reference N-11). The U.S. now produces its sulfur using the Claus process (from natural gas and petroleum). A description of the Claus sulfur production process follows. Sulfur production data are shown in Table N-3.

Table N-1

DATA FOR THE PRODUCTION OF TOLUENE DIISOCYANATE (TDI)

(Cradle-to-TDI)

(page 1 of 3)

Raw Materials	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Crude oil	314	lb	314	kg
Natural Gas	166	lb	166	kg
Salt	428	lb	428	kg
Soda Ash	4.03	lb	4.03	kg
Sulfur	2.73	lb	2.73	kg
Process water	354	gal	2,956	liter
Oxygen from air	4.06	lb	4.06	kg
Nitrogen from air	53.8	lb	53.8	kg

Energy Usage			Total Energy Thousand Btu			Total Energy GigaJoules
Energy of Material Resource						
Natural Gas			3,551			8.27
Petroleum			5,885			13.7
Total Resource			9,436			22.0
Process Energy						
Electricity (grid)	262	kwh	2,790	578	kwh	6.49
Electricity (cogeneration)	1,272	cu ft (1)	1,424	79.4	cu meters	3.32
Natural gas	6,688	cu ft	7,491	418	cu meters	17.4
LPG	0.044	gal	4.70	0.36	liter	0.011
Bit./Sbit. Coal	17.6	lb	197	17.6	kg	0.46
Distillate oil	0.78	gal	123	6.48	liter	0.29
Residual oil	2.92	gal	501	24.4	liter	1.17
Gasoline	0.041	gal	5.76	0.34	liter	0.013
Recovered Energy	351	thousand Btu	351	817	MJ	0.82
Total Process			12,186			28.4
Transportation Energy						
Combination truck	6.34	ton-miles		20.4	tonne-km	
Diesel	0.067	gal	10.6	0.56	liter	0.025
Rail	23.6	ton-miles		76.1	tonne-km	
Diesel	0.059	gal	9.31	0.49	liter	0.022
Barge	25.9	ton-miles		83.3	tonne-km	
Diesel	0.021	gal	3.29	0.17	liter	0.0076
Residual oil	0.069	gal	11.8	0.57	liter	0.027
Ocean freighter	927	ton-miles		2,982	tonne-km	
Diesel	0.18	gal	28.0	1.47	liter	0.065
Residual	1.58	gal	272	13.2	liter	0.63
Pipeline-natural gas	83.4	ton-miles		269	tonne-km	
Natural gas	57.6	cu ft	64.5	3.59	cu meter	0.15
Pipeline-petroleum products	146	ton-miles		470	tonne-km	
Electricity	3.18	kwh	32.6	7.02	kwh	0.076
Total Transportation			432			1.00

(1) The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

Table N-1

DATA FOR THE PRODUCTION
OF TOLUENE DIISOCYANATE (TDI)
(Cradle-to-TDI)
(page 2 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Environmental Emissions				
Atmospheric Emissions				
Aldehydes (unspecified)	2.4E-04	lb	2.4E-04	kg
Ammonia	0.39	lb	0.39	kg
Antimony	6.3E-07	lb	6.3E-07	kg
Arsenic	8.0E-08	lb	8.0E-08	kg
Benzene	0.016	lb	0.016	kg
Carbon Dioxide - Fossil	41.1	lb	41.1	kg
Carbon Monoxide	1.61	lb	1.61	kg
Carbon Tetrachloride	8.8E-05	lb	8.8E-05	kg
CFC 13 (Methane, trichlorofluoro-)	6.8E-06	lb	6.8E-06	kg
Chlorine	8.1E-04	lb	8.1E-04	kg
Chromium	2.1E-07	lb	2.1E-07	kg
Ethylbenzene	0.0019	lb	0.0019	kg
Ethylene Dibromide	1.3E-06	lb	1.3E-06	kg
HCFC-123	4.1E-05	lb	4.1E-05	kg
HCFC-22	0.010	lb	0.010	kg
HFC-134a	4.1E-05	lb	4.1E-05	kg
Hydrogen Chloride	0.0011	lb	0.0011	kg
NMVOC, non-methane volatile organic compounds, unspecified origin	0.21	lb	0.21	kg
Lead	1.0E-07	lb	1.0E-07	kg
Mercury	7.8E-05	lb	7.8E-05	kg
Methane	2.57	lb	2.57	kg
Nickel	1.8E-06	lb	1.8E-06	kg
Nitrogen Oxides	0.60	lb	0.60	kg
Non-Methane Hydrocarbons	0.024	lb	0.024	kg
o-Dichlorobenzene	0.0010	lb	0.0010	kg
Other Organics	0.13	lb	0.13	kg
Particulates (PM10)	0.030	lb	0.030	kg
Particulates (PM2.5)	0.0082	lb	0.0082	kg
Particulates (unspecified)	0.41	lb	0.41	kg
Phosgene	1.0E-05	lb	1.0E-05	kg
Polyaromatic Hydrocarbons (total)	1.7E-05	lb	1.7E-05	kg
Sulfur Dioxide	0.39	lb	0.39	kg
Sulfur Oxides	0.16	lb	0.16	kg
TDA	1.0E-05	lb	1.0E-05	kg
TDI	1.0E-04	lb	1.0E-04	kg
TOC	0.81	lb	0.81	kg
Toluene	0.025	lb	0.025	kg
VOC	0.13	lb	0.13	kg
Xylene	0.014	lb	0.014	kg
Solid Wastes				
Landfilled	15.1	lb	15.1	kg
Burned	1.34	lb	1.34	kg
Waste-to-Energy	34.3	lb	34.3	kg
Waterborne Wastes				
m-Xylene	3.2E-06	lb	3.2E-06	kg
1-Methylfluorene	5.0E-09	lb	5.0E-09	kg
2,4-Dimethylphenol	3.1E-06	lb	3.1E-06	kg
2-Hexanone	7.3E-07	lb	7.3E-07	kg
2-Methylnaphthalene	1.7E-06	lb	1.7E-06	kg
4-Methyl-2-Pentanone	1.8E-07	lb	1.8E-07	kg
Acetone	4.4E-07	lb	4.4E-07	kg
Acid (benzoic)	1.1E-04	lb	1.1E-04	kg
Acid (hexanoic)	2.4E-05	lb	2.4E-05	kg
Acid (unspecified)	0.0025	lb	0.0025	kg
Alkylated benzenes	2.1E-05	lb	2.1E-05	kg
Alkylated fluorenes	1.2E-06	lb	1.2E-06	kg
Alkylated naphthalenes	3.5E-07	lb	3.5E-07	kg
Alkylated phenanthrenes	1.5E-07	lb	1.5E-07	kg
Aluminum	0.010	lb	0.010	kg
Ammonia	0.034	lb	0.034	kg
Antimony	6.6E-06	lb	6.6E-06	kg
Arsenic	2.3E-05	lb	2.3E-05	kg
Barium	0.14	lb	0.14	kg
Benzene	1.3E-04	lb	1.3E-04	kg
Beryllium	1.4E-06	lb	1.4E-06	kg
BOD	0.42	lb	0.42	kg
Boron	3.5E-04	lb	3.5E-04	kg
Bromide	0.015	lb	0.015	kg
Cadmium	3.5E-06	lb	3.5E-06	kg
Calcium	0.24	lb	0.24	kg
Chlorides	2.97	lb	2.97	kg
Chloroform	1.0E-06	lb	1.0E-06	kg

Table N-1

DATA FOR THE PRODUCTION
OF TOLUENE DIISOCYANATE (TDI)
(Cradle-to-TDI)
(page 3 of 3)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Chromium (unspecified)	2.8E-04	lb	2.8E-04	kg
Cobalt	2.5E-06	lb	2.5E-06	kg
COD	0.62	lb	0.62	kg
Copper	3.2E-05	lb	3.2E-05	kg
Cyanide	3.0E-05	lb	3.0E-05	kg
Dibenzofuran	8.3E-09	lb	8.3E-09	kg
Dibenzothiophene	6.7E-09	lb	6.7E-09	kg
Dissolved Solids	24.0	lb	24.0	kg
Ethylbenzene	7.0E-06	lb	7.0E-06	kg
Fluorene	5.8E-07	lb	5.8E-07	kg
Iron	0.020	lb	0.020	kg
Lead	5.9E-05	lb	5.9E-05	kg
Lead 210	1.2E-14	lb	1.2E-14	kg
Lithium	0.025	lb	0.025	kg
Magnesium	0.048	lb	0.048	kg
Manganese	7.0E-05	lb	7.0E-05	kg
Mercury	3.8E-07	lb	3.8E-07	kg
Methyl Chloride	1.8E-09	lb	1.8E-09	kg
Methyl Ethyl Ketone	3.5E-09	lb	3.5E-09	kg
Molybdenum	2.6E-06	lb	2.6E-06	kg
Naphthalene	2.0E-06	lb	2.0E-06	kg
n-Decane	3.3E-06	lb	3.3E-06	kg
n-Docosane	4.7E-08	lb	4.7E-08	kg
n-Dodecane	6.2E-06	lb	6.2E-06	kg
n-Eicosane	1.7E-06	lb	1.7E-06	kg
n-Hexacosane	2.9E-08	lb	2.9E-08	kg
n-Hexadecane	6.7E-06	lb	6.7E-06	kg
Nickel	2.8E-05	lb	2.8E-05	kg
Nitrates	0.027	lb	0.027	kg
n-Octadecane	1.7E-06	lb	1.7E-06	kg
p -Xylene	1.2E-06	lb	1.2E-06	kg
o -Xylene	1.2E-06	lb	1.2E-06	kg
o-Cresol	3.2E-06	lb	3.2E-06	kg
o-Dichlorobenzene	1.0E-04	lb	1.0E-04	kg
Oil	0.017	lb	0.017	kg
p-Cresol	3.5E-06	lb	3.5E-06	kg
p-Cymene	4.4E-09	lb	4.4E-09	kg
Pentamethylbenzene	3.3E-09	lb	3.3E-09	kg
Phenanthrene	9.0E-08	lb	9.0E-08	kg
Phenol/ Phenolic Compounds	1.1E-04	lb	1.1E-04	kg
Phosphates	0.0010	lb	0.0010	kg
Tetradecane	2.6E-06	lb	2.6E-06	kg
Radium 226	4.1E-12	lb	4.1E-12	kg
Radium 228	2.1E-14	lb	2.1E-14	kg
Selenium	1.8E-06	lb	1.8E-06	kg
Silver	1.5E-04	lb	1.5E-04	kg
Sodium	0.70	lb	0.70	kg
Sodium Hydroxide	1.00	lb	1.00	kg
Strontium	0.0061	lb	0.0061	kg
Sulfates	0.0050	lb	0.0050	kg
Sulfides	0.0011	lb	0.0011	kg
Sulfur	2.7E-04	lb	2.7E-04	kg
Surfactants	5.9E-05	lb	5.9E-05	kg
Suspended Solids	1.25	lb	1.25	kg
Thallium	1.4E-06	lb	1.4E-06	kg
Tin	2.6E-05	lb	2.6E-05	kg
Titanium	1.0E-04	lb	1.0E-04	kg
TOC	0.010	lb	0.010	kg
Toluene	1.2E-04	lb	1.2E-04	kg
Total biphenyls	1.4E-06	lb	1.4E-06	kg
Total dibenzothiophenes	4.3E-09	lb	4.3E-09	kg
Vanadium	2.0E-05	lb	2.0E-05	kg
Xylene, unspecified	5.5E-05	lb	5.5E-05	kg
Yttrium	7.5E-07	lb	7.5E-07	kg
Zinc	2.4E-04	lb	2.4E-04	kg

References: Tables B-2 through B-5, F-3, I-2, I-3b, J-2, and N-2 through N-6.

Source: Franklin Associates, A Division of ERG models

Table N-2

DATA FOR THE PRODUCTION OF TOLUENE

	English units (Basis: 1,000 lb)		Total Energy Thousand Btu	SI units (Basis: 1,000 kg)		Total Energy GigaJoules
Material Inputs						
Naphtha (from refinery)	1,000	lb		1,000	kg	
Energy Usage						
Process Energy						
Electricity (grid)	10.8	kwh	111	23.9	kwh	0.26
Natural gas	394	cu ft	441	24.6	cu meters	1.03
Distillate oil	0.60	gal	95.2	5.00	liter	0.22
Residual oil	5.80	gal	995	48.4	liter	2.32
Total Process			1,643			3.83
Transportation Energy						
Barge	7.50	ton-miles		24.1	tonne-km	
Diesel	0.0060	gal	0.95	0.050	liter	0.0022
Residual oil	0.020	gal	3.42	0.17	liter	0.0080
Total Transportation			4.38			0.010
Environmental Emissions						
Atmospheric Emissions						
Carbon Dioxide (fossil)	45.2	lb		45.2	kg	
Carbon Monoxide	0.0051	lb		0.0051	kg	
Nitrogen Oxides	0.062	lb		0.062	kg	
Particulates	0.020	lb		0.020	kg	
Sulfur Oxides	0.44	lb		0.44	kg	
Solid Wastes						
Landfilled	0.022	lb		0.022	kg	
Waterborne Wastes						
BOD	0.70	lb		0.70	kg	
COD	1.08	lb		1.08	kg	
Dissolved solids	0.11	lb		0.11	kg	
Oil	0.018	lb		0.018	kg	
Sulfides	0.0033	lb		0.0033	kg	

References: N-3 through N-6.

Source: Franklin Associates, A Division of ERG

Table N-3

DATA FOR THE PRODUCTION OF SULFUR
(Page 1 of 2)

	English units (Basis: 1,000 lb)			SI units (Basis: 1,000 kg)		
Energy Usage			**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy						
Electricity (grid)	144	kwh	1,483	318	kwh	3.45
Natural Gas	2,123	cu ft	2,378	133	cu meters	5.54
LPG	0.15	gal	16.0	1.24	liter	0.037
Distillate Oil	0.20	gal	31.8	1.67	liter	0.074
Residual Oil	3.63	gal	623	30.3	liter	1.45
Gasoline	0.11	gal	15.2	0.89	liter	0.035
Recovered Energy	2,578	thousand Btu	2,578	5,996	MJ	6.00
Total Process			1,969			16.6
Transportation Energy						
Combination Truck	25.0	ton-miles		80.3	tonne-km	
Diesel	0.26	gal	41.6	2.19	liter	0.097
Rail	10.3	ton-miles		33.2	tonne-km	
Diesel	0.026	gal	4.06	0.21	liter	0.0095
Barge	79.8	ton-miles		257	tonne-km	
Diesel	0.064	gal	10.1	0.53	liter	0.024
Residual Ooil	0.21	gal	36.4	1.77	liter	0.085
Ocean Freighter	1,612	ton-miles		5,186	tonne-km	
Diesel	0.31	gal	48.6	2.55	liter	0.11
Residual	2.76	gal	473	23.0	liter	1.10
Pipeline-Natural Gas	94.8	ton-miles		305	tonne-km	
Natural Gas	65.4	cu ft	73.3	4.08	cu meter	0.17
Pipeline-Petroleum Products	330	ton-miles		1,062	tonne-km	
Electricity	7.19	kwh	73.6	15.9	kwh	0.17
Total Transportation			761			1.77
Environmental Emissions						
Atmospheric Emissions						
Aldehydes	0.089	lb		0.089	kg	
Ammonia	0.0038	lb		0.0038	kg	
Antimony	2.2E-06	lb		2.2E-06	kg	
Arsenic	2.8E-07	lb		2.8E-07	kg	
Benzene	0.019	lb		0.019	kg	
Carbon dioxide, fossil	217	lb		217	kg	
Carbon monoxide	3.70	lb		3.70	kg	
Carbon tetrachloride	1.3E-08	lb		1.3E-08	kg	
Methane, chlorotrifluoro-, CF	2.3E-05	lb		2.3E-05	kg	
Chromium	7.3E-07	lb		7.3E-07	kg	
Ethylbenzene	0.0023	lb		0.0023	kg	
Ethylene dibromide	4.6E-06	lb		4.6E-06	kg	
NMVOC, non-methane volatil	0.73	lb		0.73	kg	
Methane, fossil	6.82	lb		6.82	kg	
Nitrogen oxides	0.46	lb		0.46	kg	
Particulates, < 10 um	0.034	lb		0.034	kg	
Particulates, < 2.5 um	0.025	lb		0.025	kg	
Polycyclic organic matter, uns	6.0E-05	lb		6.0E-05	kg	
SO2 (original was SOx,unspeci	0.63	lb		0.63	kg	
Toluene	0.028	lb		0.028	kg	
VOC	0.15	lb		0.15	kg	
Xylene	0.017	lb		0.017	kg	
Solid Wastes						
Landfilled	39.6	lb		39.6	kg	
Waterborne Wastes						
2-Hexanone	1.9E-06	lb		1.9E-06	kg	
4-Methyl-2-Pentanone	3.5E-07	lb		3.5E-07	kg	
Acetone	8.3E-07	lb		8.3E-07	kg	
Aluminum	0.027	lb		0.027	kg	
Ammonia	0.020	lb		0.020	kg	
Antimony	1.7E-05	lb		1.7E-05	kg	
Arsenic, ion	6.0E-05	lb		6.0E-05	kg	
Barium	0.37	lb		0.37	kg	
Benzene	3.4E-04	lb		3.4E-04	kg	
Benzene, 1-methyl-4-(1-methyl	8.3E-09	lb		8.3E-09	kg	
Benzene, ethyl-	1.9E-05	lb		1.9E-05	kg	
Benzene, pentamethyl-	6.2E-09	lb		6.2E-09	kg	
Benzenes, alkylated, unspecifi	5.6E-05	lb		5.6E-05	kg	
Benzoic acid	3.0E-04	lb		3.0E-04	kg	
Beryllium	3.7E-06	lb		3.7E-06	kg	
Biphenyl	3.6E-06	lb		3.6E-06	kg	
BOD5, Biological Oxygen Dem	0.069	lb		0.069	kg	
Boron	9.1E-04	lb		9.1E-04	kg	
Bromide	0.040	lb		0.040	kg	
Cadmium, ion	9.2E-06	lb		9.2E-06	kg	
Calcium, ion	0.64	lb		0.64	kg	

Table N-3

DATA FOR THE PRODUCTION OF SULFUR
(Page 2 of 2)

	English units (Basis: 1,000 lb)		SI units (Basis: 1,000 kg)	
Chlorides	7.85	lb	7.85	kg
Chromium	7.4E-04	lb	7.4E-04	kg
Cobalt	6.4E-06	lb	6.4E-06	kg
COD, Chemical Oxygen Demar	0.30	lb	0.30	kg
Copper, ion	8.0E-05	lb	8.0E-05	kg
Cyanide	6.0E-09	lb	6.0E-09	kg
Decane	8.4E-06	lb	8.4E-06	kg
Dibenzofuran	1.6E-08	lb	1.6E-08	kg
Dibenzothiophene	1.3E-08	lb	1.3E-08	kg
Dissolved solids	8.28	lb	8.28	kg
Docosane	8.9E-08	lb	8.9E-08	kg
Dodecane	1.6E-05	lb	1.6E-05	kg
Eicosane	4.4E-06	lb	4.4E-06	kg
Florene, 1-methyl-	9.5E-09	lb	9.5E-09	kg
Florenes, alkylated, unspecifie	3.2E-06	lb	3.2E-06	kg
Fluorine	1.5E-06	lb	1.5E-06	kg
Hexadecane	1.7E-05	lb	1.7E-05	kg
Hexanoic acid	6.1E-05	lb	6.1E-05	kg
Iron	0.051	lb	0.051	kg
Lead	1.5E-04	lb	1.5E-04	kg
Lead-210/kg	3.0E-14	lb	3.0E-14	kg
Lithium, ion	0.029	lb	0.029	kg
Magnesium	0.13	lb	0.13	kg
Manganese	1.9E-04	lb	1.9E-04	kg
Mercury	3.7E-07	lb	3.7E-07	kg
Methane, monochloro-, R-40	3.4E-09	lb	3.4E-09	kg
Methyl Ethyl Ketone	6.7E-09	lb	6.7E-09	kg
Molybdenum	6.7E-06	lb	6.7E-06	kg
m-Xylene	8.3E-06	lb	8.3E-06	kg
Naphthalene	5.2E-06	lb	5.2E-06	kg
Naphthalenes, alkylated, unsp	9.2E-07	lb	9.2E-07	kg
Napthalene, 2-methyl-	4.4E-06	lb	4.4E-06	kg
n-Hexacosane	5.6E-08	lb	5.6E-08	kg
Nickel	7.0E-05	lb	7.0E-05	kg
o-Cresol	8.4E-06	lb	8.4E-06	kg
Octadecane	4.3E-06	lb	4.3E-06	kg
Oils, unspecified	0.017	lb	0.017	kg
o-xylene	3.1E-06	lb	3.1E-06	kg
p-Cresol	9.0E-06	lb	9.0E-06	kg
Phenanthrene	2.3E-07	lb	2.3E-07	kg
Phenanthrenes, alkylated, uns	3.8E-07	lb	3.8E-07	kg
Phenol, 2,4-dimethyl-	8.2E-06	lb	8.2E-06	kg
Phenols, unspecified	3.4E-04	lb	3.4E-04	kg
p-xylene	3.1E-06	lb	3.1E-06	kg
Radium-226/kg	1.1E-11	lb	1.1E-11	kg
Radium-228/kg	5.4E-14	lb	5.4E-14	kg
Selenium	5.0E-06	lb	5.0E-06	kg
Silver	4.0E-04	lb	4.0E-04	kg
Sodium, ion	1.89	lb	1.89	kg
Strontium	0.016	lb	0.016	kg
Sulfate	0.014	lb	0.014	kg
Sulfides	2.0E-04	lb	2.0E-04	kg
Sulfur	7.0E-04	lb	7.0E-04	kg
Surfactants, unspecified	1.6E-04	lb	1.6E-04	kg
Suspended solids, unspecified	3.06	lb	3.06	kg
Tetradecane	6.7E-06	lb	6.7E-06	kg
Thallium	3.6E-06	lb	3.6E-06	kg
Tin	6.8E-05	lb	6.8E-05	kg
Titanium, ion	2.6E-04	lb	2.6E-04	kg
Toluene	3.1E-04	lb	3.1E-04	kg
Vanadium	6.5E-05	lb	6.5E-05	kg
Xylene	1.5E-04	lb	1.5E-04	kg
Yttrium	1.9E-06	lb	1.9E-06	kg
Zinc	6.2E-04	lb	6.2E-04	kg

References: N-15 through N-17.

Source: Franklin Associates, A Division of ERG

Recovery of sulfur from sour natural gas and crude oil via the Claus process accounts for the total amount of the sulfur produced in the United States. Approximately 79 percent of the sulfur produced via Claus recovery is obtained from hydrogen sulfide recovered from petroleum refining, and the remaining 21 percent is recovered from natural gas sweetening (Reference N-11). The following data includes data for the production of sulfur from petroleum refining only.

Hydrogen sulfide is recovered from refinery gases by absorption in a solvent or by regenerative chemical absorption (Reference N-12). Hydrogen sulfide concentrations in the gas from the absorption unit vary. For this analysis, an industry average H2S gas concentration of 85 percent is used (References N-13 and N-12). This concentrated hydrogen sulfide stream is treated by the Claus process to recover the sulfur. The Claus process is based upon the reaction of hydrogen sulfide with sulfur dioxide according to the exothermic reaction (Reference N-12):

$$2H2S + SO2 \rightarrow 3S + 2H2O \qquad \text{(Reaction 1)}$$

Sulfur dioxide for the reaction is prepared by oxidation of hydrogen sulfide with air or oxygen in a furnace using either the partial combustion process (once-through process) or the split-stream process. The partial combustion method is used when the H2S concentration is greater than 50 percent and the hydrocarbon concentration is less than 2 percent. The split stream process is used when there is an H2S concentration of 20 to 50 percent and a hydrocarbon concentration of less than 5 percent.

In the partial combustion method, the hydrogen sulfide-rich gas stream is burned with a fuel gas in an oxygen-limited environment to oxidize one-third of the H2S to SO2 according to the reaction (Reference N-14):

$$2H2S + 2O2 \rightarrow SO2 + S + 2H2O \qquad \text{(Reaction 2)}$$

Sulfur is removed from the burner and the H2S/SO2 mixture moves to the catalytic converter chambers.

In the split stream process, one-third of the hydrogen sulfide is split off and completely oxidized to SO_2 according to the reaction:

$$2H_2S + 3O_2 \rightarrow 2SO_2 + 2H_2O \qquad \text{(Reaction 3)}$$

The remaining two-thirds of the H_2S is mixed with the combustion product and enters the catalytic converter chambers.

The H_2S and SO_2 mixture from either process is passed through one or more catalyst beds and is converted to sulfur, which is removed by condensers between each bed. For this analysis, an H_2S concentration of 85 percent has been assumed; therefore, it is also assumed that the partial combustion process is used.

Although efficiencies of 96 to 99 percent sulfur recovery have been demonstrated for the Claus process, recovery is usually not over 96 percent and is limited by thermodynamic considerations (References N-12 and N-14). For this analysis, a sulfur recovery efficiency of 95 percent is assumed.

The energy generated from burning hydrogen sulfide to produce SO_2 is usually recovered and used directly to reheat the process stream in secondary and tertiary condensers, or recovered as steam for use in other processes (Reference N-14). Heat released from cooling the exothermic reaction to form sulfur is also recovered.

Sulfuric Acid Production

All sulfuric acid produced in the U.S. is produced by the contact process (Reference N-20). The sulfur input streams used by contact plants can be of three different forms: (1) elemental sulfur, (2) spent sulfuric acid or hydrogen sulfides, and (3) metal sulfide ores or smelter gas. Contact plants that use elemental sulfur account for 81 percent of sulfuric acid production (Reference N-18).

There are three basic steps in the contact process. The first step oxidizes (burns) sulfur to sulfur dioxide (SO_2). The second step catalytically oxidizes sulfur dioxide to sulfur trioxide (SO_3). The third step dissolves the sulfur trioxide into a 98 percent solution of sulfuric acid. The third step can also produce sulfuric acid by adding sulfur trioxide directly to water. However, when sulfur trioxide is added directly to water, the reaction is slow and tends to form a mist.

During sulfuric acid production, the burning of sulfur produces heat, which in turn is used to generate steam. This steam is usually used in adjacent processing plants and supplies energy to the sulfuric acid plant. The exported steam is given a credit and shown as recovered energy.

Process data for sulfuric acid production are shown in Table N-4.

Table N-4

DATA FOR THE PRODUCTION
OF SULFURIC ACID

	English units (Basis: 1,000 lb)		Total Energy Thousand Btu	SI units (Basis: 1,000 kg)		Total Energy GigaJoules
Material Inputs						
Sulfur	330	lb		330	kg	
Water	183	lb		183	kg	
Oxygen from air	489	lb		489	kg	
Energy Usage						
Process Energy						
Electricity (grid)	30.0	kwh	309	66.1	kwh	0.72
Recovered Energy	850	thousand Btu	850	1,977	MJ	1.98
Total Process			-541			-1.26
Transportation Energy						
Combination Truck	7.50	ton-miles		24.1	tonne-km	
Diesel	0.079	gal	12.5	0.66	liter	0.029
Total Transportation			12.5			0.029
Environmental Emissions						
Atmospheric Emissions						
Nitrogen Oxides	0.050	lb		0.050	kg	
Particulates (unspecified)	1.00	lb		1.00	kg	
Sulfur Oxides	2.59	lb		2.59	kg	
Solid Wastes						
Landfilled	0.50	lb		0.50	kg	
Waterborne Wastes						
Acid (unspecified)	0.30	lb		0.30	kg	
BOD	0.10	lb		0.10	kg	
Suspended Solids	0.30	lb		0.30	kg	

References: N-5, N-19, and N-21.

Source: Franklin Associates, A Division of ERG

Soda Ash Mining & Processing

Soda ash used in the U.S. is naturally occurring and is obtained from trona and alkaline brines in the Green River basin in Wyoming and Searles Lake in California. The soda ash is mined using two different methods, underground trona mining and solution mining. Underground trona mining is similar to coal mining. The most common methods are the room and pillar method and the long wall method. In both of these processes, the material is undercut, drilled, blasted, crushed, and then transported to the surface. Solution mining is currently used by one of the six major soda ash producers in the U.S. (Reference N-23). Soda ash from solution mining is for the most part used for the manufacture of caustic soda. The data in this module are based on underground trona mining.

After mining, trona is crushed, screened and then calcined in rotary, gas-fired kilns. The mineral is then dissolved in water and filtered. The resulting soda ash solution (sodium carbonate) is evaporated and dried (Reference N-20). Airborne particulates generated from mining and drying operations are reduced by control equipment such as bag filters and wet scrubbers. Airborne carbon dioxide is generated from calcining operations. Solid wastes and water effluents generated during soda ash mining and production are recycled to the soda ash treatment processes, held in on-site evaporation ponds, or are returned to mine-shaft voids. Due to the onsite treatment of solid and waterborne wastes, this module assumes that negligible solid wastes and water emissions are produced from soda ash production and released to the environment (References N-5 and N-20).

Soda ash can also be produced synthetically via the Solvay process. The Solvay process uses salt, coke, limestone, with ammonia as a catalyst. Synthetic soda ash is more expensive to produce than natural soda ash and also has high concentrations of calcium chloride and sodium chloride in the process effluent. This method of soda ash production is not currently used in the U.S.

U.S. production provides nearly all of the soda ash required by U.S. manufacturers. Approximately 45 percent of the total soda ash manufactured is used in glass manufacturing. Soda ash mining and processing data are shown in Table N-5.

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 nitric acid and nitro compounds is recycled (Reference N-8).

Sulfuric acid is separated and recycled back into the production of nitroaromatics. Since the 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 in the United States. This data was aggregated with phosgene, TDA, and TDI and is included in Table N-6.

Table N-5

DATA FOR THE MINING & PROCESSING OF SODA ASH

Energy Usage	English units (Basis: 1,000 lb)		Total Energy Thousand Btu	SI units (Basis: 1,000 kg)		Total Energy GigaJoules
Process Energy						
Electricity (grid)	41.1	kwh	423	90.6	kwh	0.98
Natural gas	797	cu ft	893	49.8	cu meters	2.08
Coal	108	lb	1,213	108	kg	2.82
Distillate oil	0.067	gal	10.6	0.067	liter	0.025
Residual oil	0.19	gal	32.6	1.59	liter	0.076
Total Process			2,572			5.99
Transportation Energy						
Combination truck	7.50	ton-miles		24.1	tonne-km	
Diesel	0.079	gal	12.5	0.66	liter	0.029
Total Transportation			12.5			0.029
Environmental Emissions						
Atmospheric Emissions						
Carbon Dioxide (fossil)	415	lb		415	kg	
Particulates (unspecified)	96.5	lb		96.5	kg	

References: N-5, N-20, and N-22.

Source: Franklin Associates, A Division of ERG

Toluene Diamine (TDA) Production

Toluene Diamine (TDA) is produced by the hydrogenation of dinitrotoluene. The catalytic hydrogenation of dinitrotoluene to toluene diamine is a standard aromatic synthesis process. The isomer ratio for TDA depends on the DNT isomer ratio used. Water, toluidine, and ortho-TDA can be removed by distillation or will be separated after phosgenation with the TDI residue (Reference N-8).

Because confidential datasets cannot be shown individually, the datasets for DNT, phosgene, TDA, and TDI were combined into one data table. TDA data was collected from two sources and are included with the TDI energy and emissions in Table N-6. The TDA producers verified that the characteristics of their plants are representative of a majority of North American TDA production. The average DNT/phosgene/TDA/TDI dataset was reviewed and accepted by all DNT/phosgene/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 reacted with excess phosgene to produce the TDI. After phosgenation, the mixture is stripped from the solvent and separated by distillation (Reference N-9). 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 today the most important commercial product, but other mixtures are available.

Table N-6 presents the data for the production of DNT, phosgene, TDA, and TDI. Data for the production of phosgene, TDA, and TDI were provided by three leading producers (3 plants) in North America to Franklin Associates. Heat was exported as a coproduct for some producers. The energy amount for the exported heat was reported separately as recovered energy. A large amount of hydrogen chloride is produced as a coproduct during this process. A mass basis was used to partition the credit for each product. The coproduct amount is not shown due to confidentiality issues. 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. Confidentiality issues prohibit the revealing of each plant's individual HCl coproduct amount. An average of the coproduct could be provided, but this would not allow for precise reproduction of the dataset.

As of 2002 there were 5 TDI producers and 6 TDI plants in the U.S. (Reference N-1 and N-2). The TDI data collected represents approximately half of the total North American TDI production amount. The TDI producers who provided data for this module verified that the characteristics of their plants are representative of a majority of North American TDI production. The average dataset was reviewed and accepted by all TDI data providers.

To assess the quality of the data collected for TDI, the collection methods, 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 engineering estimates. All data submitted for TDI represents the year 2003 and represents U.S. production.

Table N-6

DATA FOR THE PRODUCTION OF TOLUENE DIISOCYANATE (TDI)

(Includes Dinitrotoluene, Phosgene and TDA)

	English units (Basis: 1,000 lb)				SI units (Basis: 1,000 kg)		
Material Inputs							
Carbon Monoxide	192	lb			192	kg	
Chlorine	462	lb			462	kg	
Sodium Hydroxide	22.6	lb			22.6	kg	
Toluene	308	lb			308	kg	
Nitric Acid	431	lb			431	kg	
Sulfuric Acid	8.26	lb			8.26	kg	
Soda Ash	4.03	lb			4.03	kg	
Energy Usage				**Total Energy Thousand Btu**			**Total Energy GigaJoules**
Process Energy							
Electricity (grid)	29.5	kwh		303	65.0	kwh	0.71
Electricity (cogeneration)	768	cu ft	(1)	860	47.9	cu meters	2.00
Natural gas	3,991	cu ft		4,470	249	cu meters	10.4
Recovered Energy	337	thousand Btu		337	784	MJ	0.78
Total Process				5,296			12.3
Transportation Energy							
Ocean freighter	753	ton-miles			2,422	tonne-km	
Diesel	0.14	gal		22.7	1.19	liter	0.053
Residual	1.29	gal		221	10.7	liter	0.51
Pipeline-petroleum products	0.36	ton-miles			1.16	tonne-km	
Electricity	0.0078	kwh		0.080	0.017	kwh	1.9E-04
Total Transportation				244			0.57
Environmental Emissions							
Atmospheric Emissions							
Ammonia	0.049	lb			0.049	kg	
Carbon Monoxide	0.010	lb			0.010	kg	
Chlorine	2.8E-04	lb			2.8E-04	kg	
HFC-22	0.010	lb	(2)		0.010	kg	
Hydrochloric Acid	0.0010	lb	(2)		0.0010	kg	
Lead	1.0E-07	lb	(2)		1.0E-07	kg	
Mercury	1.0E-07	lb	(2)		1.0E-07	kg	
NM Hydrocarbons	0.024	lb			0.024	kg	
Nitrogen Oxides	0.12	lb			0.12	kg	
o-Dichlorobenzene	0.0010	lb	(2)		0.0010	kg	
Other Organics	1.0E-04	lb	(2)		1.0E-04	kg	
Particulates (unknown)	0.0057	lb			0.0057	kg	
PM2.5	0.0010	lb	(2)		0.0010	kg	
PM10	0.011	lb			0.011	kg	
Phosgene	1.0E-05	lb	(2)		1.0E-05	kg	
TDA	1.0E-05	lb	(2)		1.0E-05	kg	
TDI	1.0E-04	lb	(2)		1.0E-04	kg	
VOC	1.0E-04	lb	(2)		1.0E-04	kg	
Solid Wastes							
Landfilled	0.14	lb			0.14	kg	
Burned	0.70	lb			0.70	kg	
Waste-to-Energy	34.3	lb			34.3	kg	
Waterborne Wastes							
Ammonia	1.0E-04	lb	(2)		1.0E-04	kg	
BOD	0.050	lb			0.050	kg	
Chloroform	1.0E-06	lb	(2)		1.0E-06	kg	
COD	0.17	lb			0.17	kg	
Copper	1.0E-06	lb	(2)		1.0E-06	kg	
Cyanide	3.0E-05	lb			3.0E-05	kg	
Dissolved solids	1.00	lb	(2)		1.00	kg	
Nickel	1.0E-06	lb	(2)		1.0E-06	kg	
o-Dichlorobenzene	1.0E-04	lb	(2)		1.0E-04	kg	
Phosphates	0.0010	lb	(2)		0.0010	kg	
Sodium Hydroxide	1.00	lb	(2)		1.00	kg	
Suspended Solids	0.037	lb			0.037	kg	
TOC	0.010	lb	(2)		0.010	kg	
Nitrate	0.010	lb	(2)		0.010	kg	

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(1) Fuel use for electricity from cogeneration is shown within the natural gas amount. The electricity amount from cogeneration is assumed to be produced from natural gas at a 50% efficiency.

(2) This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

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Source: Franklin Associates, A Division of ERG

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