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EPA Office of Compliance Sector Notebook Project

Profile of the Organic Chemical Industry
2nd Edition

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Office of Compliance
Office of Enforcement and Compliance Assurance
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This report is one in a series of volumes published by the U.S. Environmental Protection Agency (EPA) to provide information of general interest regarding environmental issues associated with specific industrial sectors. The documents were developed under contract by Abt Associates (Cambridge, MA), GeoLogics Corporation (Alexandria, VA), Science Applications International Corporation (McLean, VA), and Booz-Allen & Hamilton, Inc. (McLean, VA). A listing of available Sector Notebooks is included on the following page.

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The Sector Notebooks were developed by the EPA's Office of Compliance. Direct general questions about the Sector Notebook Project to:

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For further information, and for answers to questions pertaining to these documents, please refer to the contacts listed on the following page.

AVAILABLE SECTOR NOTEBOOKS

Questions and comments regarding the individual documents should be directed to Compliance Assistance and Sector Programs Division at 202 564-2310 unless otherwise noted below. **See the Notebook web page at: http://www.epa.gov/compliance/resources/publications/assistance/sectors/notebooks/ for the most recent titles and links to refreshed data.**

EPA Publication Number	Industry
EPA/310-R-95-001.	Profile of the Dry Cleaning Industry
EPA/310-R-95-002.	Profile of the Electronics and Computer Industry*
EPA/310-R-95-003.	Profile of the Wood Furniture and Fixtures Industry
EPA/310-R-95-004.	Profile of the Inorganic Chemical Industry*
EPA/310-R-95-005.	Profile of the Iron and Steel Industry
EPA/310-R-95-006.	Profile of the Lumber and Wood Products Industry
EPA/310-R-95-007.	Profile of the Fabricated Metal Products Industry*
EPA/310-R-95-008.	Profile of the Metal Mining Industry
EPA/310-R-95-009.	Profile of the Motor Vehicle Assembly Industry
EPA/310-R-95-010.	Profile of the Nonferrous Metals Industry
EPA/310-R-95-011.	Profile of the Non-Fuel, Non-Metal Mining Industry
EPA/310-R-02-001.	Profile of the Organic Chemical Industry, 2nd Edition*
EPA/310-R-95-013.	Profile of the Petroleum Refining Industry
EPA/310-R-95-014.	Profile of the Printing Industry
EPA/310-R-02-002.	Profile of the Pulp and Paper Industry, 2nd Edition
EPA/310-R-95-016.	Profile of the Rubber and Plastic Industry
EPA/310-R-95-017.	Profile of the Stone, Clay, Glass, and Concrete Ind.
EPA/310-R-95-018.	Profile of the Transportation Equipment Cleaning Ind.
EPA/310-R-97-001.	Profile of the Air Transportation Industry
EPA/310-R-97-002.	Profile of the Ground Transportation Industry
EPA/310-R-97-003.	Profile of the Water Transportation Industry
EPA/310-R-97-004.	Profile of the Metal Casting Industry
EPA/310-R-97-005.	Profile of the Pharmaceuticals Industry
EPA/310-R-97-006.	Profile of the Plastic Resin and Man-made Fiber Ind.
EPA/310-R-97-007.	Profile of the Fossil Fuel Electric Power Generation Industry
EPA/310-R-97-008.	Profile of the Shipbuilding and Repair Industry
EPA/310-R-97-009.	Profile of the Textile Industry
EPA/310-R-97-010.	Sector Notebook Data Refresh-1997 **
EPA/310-R-98-001.	Profile of the Aerospace Industry
EPA/310-R-00-001.	Profile of the Agricultural Crop Production Industry Contact: Ag Center, (888) 663-2155
EPA/310-R-00-002.	Profile of the Agricultural Livestock Production Industry Contact: Ag Center, (888) 663-2155
EPA/310-R-00-003.	Profile of the Agricultural Chemical, Pesticide and Fertilizer Industry Contact: Agriculture Division, 202 564-2320
EPA/310-R-00-004.	Profile of the Oil and Gas Extraction Industry
	Government Series
EPA/310-R-99-001.	Profile of Local Government Operations

* Spanish translations available of 1st Editions in electronic format only.

** This document revises compliance, enforcement, and toxic release inventory data for all previously published profiles. Visit the Sector Notebook web page to access the most current data.

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Organic Chemical Industry
(SIC 2861, 2865, and 2869)

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LIST OF ACRONYMS

AFS	AIRS Facility Subsystem (CAA database)
AIRS	Aerometric Information Retrieval System (CAA database)
AOR	Area of Review (SDWA)
BAT	Best Available Technology Economically Achievable
BCT	Best Conventional Pollutant Control Technology
BIFs	Boilers and Industrial Furnaces (RCRA)
BMP	Best Management Practice
BOD	Biochemical Oxygen Demand
BPT	Best Practicable Technology Currently Available
CAA	Clean Air Act
CAAA	Clean Air Act Amendments of 1990
CERCLA	Comprehensive Environmental Response, Compensation and Liability Act
CERCLIS	CERCLA Information System
CFCs	Chlorofluorocarbons
CFR	Code of Federal Regulations
CGP	Construction General Permit (CWA)
CO	Carbon Monoxide
CO_2	Carbon Dioxide
COD	Chemical Oxygen Demand
CSI	Common Sense Initiative
CWA	Clean Water Act
CZMA	Coastal Zone Management Act
D&B	Dun and Bradstreet Marketing Index
DOC	United States Department of Commerce
DPCC	Discharge Prevention, Containment and Countermeasures
EIS	Environmental Impact Statement
EPA	United States Environmental Protection Agency
EPCRA	Emergency Planning and Community Right-to-Know Act
ESA	Endangered Species Act
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
FINDS	Facility Indexing System
FR	Federal Register
FRP	Facility Response Plan
HAPs	Hazardous Air Pollutants (CAA)
HSDB	Hazardous Substances Data Bank
HSWA	Hazardous and Solid Waste Amendments
IDEA	Integrated Data for Enforcement Analysis
LDR	Land Disposal Restrictions (RCRA)
LEPCs	Local Emergency Planning Committees
MACT	Maximum Achievable Control Technology (CAA)
MCLGs	Maximum Contaminant Level Goals
MCLs	Maximum Contaminant Levels
MEK	Methyl Ethyl Ketone

MSDSs	Material Safety Data Sheets
MSGP	Multi-Sector General Permit (CWA)
NAAQS	National Ambient Air Quality Standards (CAA)
NAFTA	North American Free Trade Agreement
NAICS	North Americal Industrial Classification System
NCDB	National Compliance Database (for TSCA, FIFRA, EPCRA)
NCP	National Oil and Hazardous Substances Pollution Contingency Plan
NEC	Not Elsewhere Classified
NEIC	National Enforcement Investigations Center
NEPA	National Environmental Policy Act
NESHAP	National Emission Standards for Hazardous Air Pollutants
$NICE^3$	National Industrial Competitiveness Through Energy, Environment and Economics
NO_2	Nitrogen Dioxide
NOI	Notice of Intent
NOT	Notice of Termination
NOV	Notice of Violation
NO_x	Nitrogen Oxides
NPDES	National Pollution Discharge Elimination System (CWA)
NPL	National Priorities List
NRC	National Response Center
NSPS	New Source Performance Standards (CAA)
OAQPS	Office of Air Quality Planning and Standards
OAR	Office of Air and Radiation
OECA	Office of Enforcement and Compliance Assurance
OMB	Office of Management and Budget
OPA	Oil Pollution Act
OPPTS	Office of Prevention, Pesticides, and Toxic Substances
OSHA	Occupational Safety and Health Administration
OSW	Office of Solid Waste
OSWER	Office of Solid Waste and Emergency Response
OW	Office of Water
P2	Pollution Prevention
PCS	Permit Compliance System (CWA Database)
PM10	Particulate Matter of 10 microns or less
PMN	Premanufacture Notice
POTW	Publicly Owned Treatments Works
PSD	Prevention of Significant Deterioration (CAA)
PT	Total Particulates
RCRA	Resource Conservation and Recovery Act
RCRIS	RCRA Information System
RQ	Reportable Quantity (CERCLA)
SARA	Superfund Amendments and Reauthorization Act
SDWA	Safe Drinking Water Act
SEPs	Supplementary Environmental Projects
SERCs	State Emergency Response Commissions
SIC	Standard Industrial Classification

SIP	State Implementation Plan
SO_2	Sulfur Dioxide
SO_x	Sulfur Oxides
SOCMI	Synthetic Organic Chemical Manufacturing Industry
SPCC	Spill Prevention Control and Countermeasures
STEP	Strategies for Today's Environmental Partnership
SWPPP	Storm Water Pollution Prevention Plan (CWA)
TOC	Total Organic Carbon
TRI	Toxic Release Inventory
TRIS	Toxic Release Inventory System
TCRIS	Toxic Chemical Release Inventory System
TSCA	Toxic Substances Control Act
TSD	Treatment Storage and Disposal
TSP	Total Suspended Particulates
TSS	Total Suspended Solids
UIC	Underground Injection Control (SDWA)
USDW	Underground Sources of Drinking Water (SDWA)
UST	Underground Storage Tanks (RCRA)
VOCs	Volatile Organic Compounds

I. INTRODUCTION TO THE SECTOR NOTEBOOK PROJECT

I.A. Summary of the Sector Notebook Project

Environmental policies based upon comprehensive analysis of air, water and land pollution (such as economic sector, and community-based approaches) are an important supplement to traditional single-media approaches to environmental protection. Environmental regulatory agencies are beginning to embrace comprehensive, multi-statute solutions to facility permitting, compliance assurance, education/outreach, research, and regulatory development issues. The central concepts driving the new policy direction are that pollutant releases to each environmental medium (air, water and land) affect each other, and that environmental strategies must actively identify and address these interrelationships by designing policies for the "whole" facility. One way to achieve a whole facility focus is to design environmental policies for similar industrial facilities. By doing so, environmental concerns that are common to the manufacturing of similar products can be addressed in a comprehensive manner. Recognition of the need to develop the industrial "sector-based" approach within the EPA Office of Compliance led to the creation of this document.

The Sector Notebook Project was initiated by the Office of Compliance within the Office of Enforcement and Compliance Assurance (OECA) to provide its staff and managers with summary information for eighteen specific industrial sectors. As other EPA offices, states, the regulated community, environmental groups, and the public became interested in this project, the scope of the original project was expanded. The ability to design comprehensive, common sense environmental protection measures for specific industries is dependent on knowledge of several interrelated topics. For the purposes of this project, the key elements chosen for inclusion are: general industry information (economic and geographic); a description of industrial processes; pollution outputs; pollution prevention opportunities; federal statutory and regulatory framework; compliance history; and a description of partnerships that have been formed between regulatory agencies, the regulated community and the public.

For any given industry, each topic listed above could alone be the subject of a lengthy volume. However, in order to produce a manageable document, this project focuses on providing summary information for each topic. This format provides the reader with a synopsis of each issue, and references where more in-depth information is available. Text within each profile was researched from a variety of sources, and was usually condensed from more detailed sources pertaining to specific topics. This approach allows for a wide coverage of activities that can be further explored based upon the references listed at the end of this profile. As a check on the information included, each notebook went through an external document review process. The Office of Compliance appreciates the efforts of all those that participated in this process and enabled us to develop more complete, accurate and up-to-date summaries. Many of those who reviewed this notebook are listed as contacts in Section IX and may be sources of additional information. The individuals and groups on this list do not necessarily concur with all statements within this notebook.

I.B. Additional Information

Providing Comments

OECA's Office of Compliance plans to periodically review and update the notebooks and will make these updates available both in hard copy and electronically. If you have any comments on the existing notebook, or if you would like to provide additional information, please send a hard copy and computer disk to the EPA Office of Compliance, Sector Notebook Project (2224-A), 1200 Pennsylvania Ave., NW, Washington, DC 20460. Comments can also be sent via the Sector Notebooks web page at: http://www.epa.gov/compliance/resources/publications/assistance/sectors/notebooks/. If you are interested in assisting in the development of new Notebooks, or if you have recommendations on which sectors should have a Notebook, please contact the Office of Compliance at 202-564-2310.

Adapting Notebooks to Particular Needs

The scope of the industry sector described in this notebook approximates the national occurrence of facility types within the sector. In many instances, industries within specific geographic regions or states may have unique characteristics that are not fully captured in these profiles. The Office of Compliance encourages state and local environmental agencies and other groups to supplement or re-package the information included in this notebook to include more specific industrial and regulatory information that may be available. Additionally, interested states may want to supplement the "Summary of Applicable Federal Statutes and Regulations" section with state and local requirements. Compliance or technical assistance providers may also want to develop the "Pollution Prevention" section in more detail.

II. INTRODUCTION TO THE ORGANIC CHEMICALS INDUSTRY

This section provides background information on the size, geographic distribution, employment, production, sales, and economic condition of the organic chemical industry. The type of facilities described within the document are also described in terms of their Standard Industrial Classification (SIC) codes.

II.A. Introduction, Background, and Scope of the Notebook

The chemical manufacturing industry (SIC 28) produces an enormous number of materials. EPA estimates that there are 15,000 chemicals manufactured in the U.S. in quantities greater than 10,000 pounds (EPA, 2002). The organic chemicals industry, which manufactures carbon-containing chemicals, accounts for much of this diversity.

The general structure of the chemical industry is displayed in Table 1. The organic and inorganic chemicals industries obtain raw materials (from petroleum and mined products, respectively) and convert them to intermediate materials or basic finished chemicals. The remaining industries in SIC 28 convert intermediate materials into a spectrum of specialized finished products.

Table 1: Structure of the Chemical Industry (SIC 28)

SIC Code	Industry Sector
281	Inorganic chemicals
282	Plastics materials and synthetics
283	Drugs
284	Soaps, cleaners, and toilet goods
285	Paints and allied products
286	*Organic chemicals*
287	Agricultural chemicals
289	Miscellaneous chemical products

This sector notebook addresses the organic chemicals industry (SIC 286). The industry is divided into three categories: gum and wood chemicals, cyclic organic crudes & intermediates, and industrial organic chemicals not elsewhere classified.

Gum and wood chemicals (SIC 2861) are materials that are distilled or otherwise separated from wood. The most common products of the industry are charcoal, tall oil, rosin, turpentine, pine tar, acetic acid, and methanol. Because the products are wood-based, many of the major producers are in the pulp and paper industry (Kline & Co., 1999).

Cyclic organic crudes and intermediates (SIC 2865) are materials processed from petroleum, natural gas, and coal. Important products include benzene, toluene, xylene, and naphthalene. Typically these products are consumed by downstream industries included in Table 1. Manufacturers of synthetic dyes and organic pigments also are included in this SIC code (U.S. Department of Labor, 2001).

Industrial organic chemicals, not elsewhere classified (SIC 2869) is by far the largest and most diverse component of the organic chemicals industry. Its products may be either intermediates or end products.

SIC codes were established by the Office of Management and Budget (OMB) to track the flow of goods and services within the economy. OMB has changed the SIC code system to a system based on similar production processes called the North American Industrial Classification System (NAICS). Because most of the data presented in this notebook apply to the organic chemicals industry as defined by its SIC codes, this notebook continues to use the SIC system to define this sector. Table 2 presents the SIC codes for the organic chemistry industry and the corresponding NAICS codes.

Table 2: SIC and NAICS Codes for the Organic Chemicals Industry

1987 SIC	SIC Description	1997 NAICS	NAICS Description
2861	Gum & wood chemicals	325191	Gum & wood chemical mfg
2865	Cyclic crudes & intermediate	325110	Petrochemical mfg (part)
		325132	Synthetic organic dye & pigment mfg
		325192	Cyclic crude & intermediate mfg
2869	Industrial organic chemicals, not elsewhere classified	325110	Petrochemical mfg (part)
		325120	Industrial gas mfg (part)
		325188	All other basic inorganic chemical mfg (part)
		325193	Ethyl alcohol mfg
		325199	All other basic organic chemical mfg (part)

Source: U.S. Census Bureau, 2000.

II.B. Characterization of the Organic Chemicals Industry

II.B.1. Product Characterization

The chemical industry produces many materials that are essential to the economy and to modern life: plastics, pharmaceuticals, and agricultural chemicals are some examples. Although these end products have very different characteristics, they are created from a relatively small number of raw materials. The organic chemicals industry, as described in this notebook, converts these raw materials into intermediate materials that are necessary to create desired end products.

The industrial organic chemical market has two broadly defined categories: commodity and specialty. Commodity chemical manufacturers compete on price and produce large volumes of small sets of chemicals using dedicated equipment with continuous and efficient processing. Specialty chemical manufacturers cater to custom markets, manufacture a diverse set of chemicals, use two or three different reaction steps to produce a product, tend to use batch processes, compete on technological expertise and have a greater value added to their products. Commodity chemical manufacturers have lower labor requirements per volume and require less professional labor per volume.

Common inputs, or feedstocks, for the industry are supplied by petroleum refiners: ethylene, propylene, benzene, methanol, toluene, xylene, butadiene, and butylene (Szmant, 1989). As noted previously, other feedstocks come from coal, natural gas, and wood. By using several processes outlined in Section III, a range of chemicals are produced from these feedstocks. Table 3 presents common categories of products and their typical end uses.

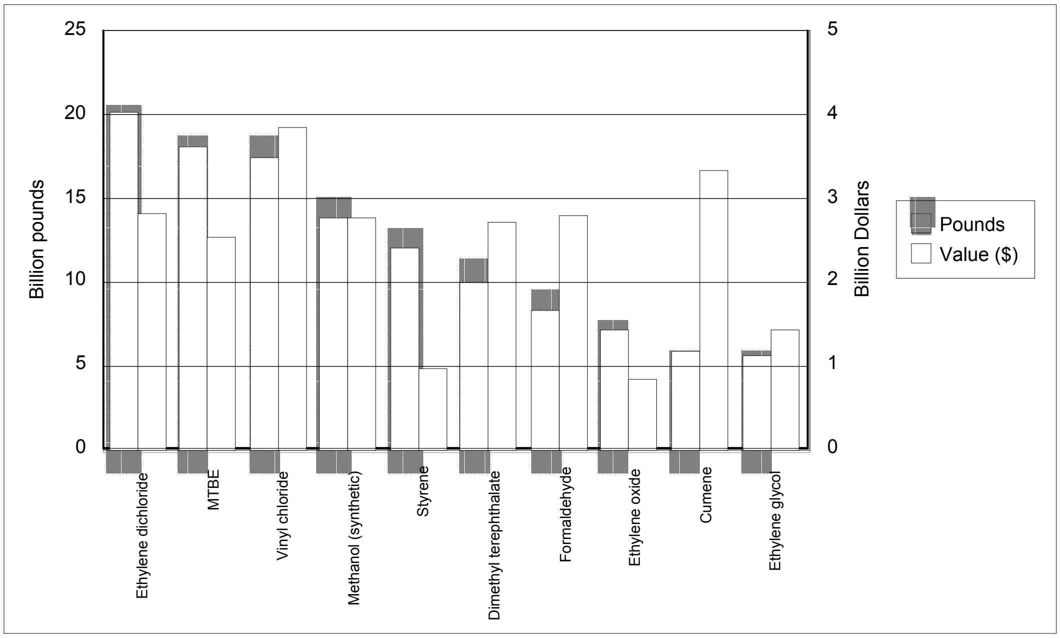
Table 3: Summary of Major Organic Chemical Products

Category	Example Chemicals	Example End Uses
Aliphatic and other acyclic organic chemicals	Ethylene, butylene, and formaldehyde	Polyethylene plastic, plywood
Solvents	Butyl alcohol, ethyl acetate, ethylene glycol ether, perchloroethylene	Degreasers, dry cleaning fluid
Polyhydric alcohols	Ethylene glycol, sorbitol, synthetic glycerin	Antifreeze, soaps
Synthetic perfume and flavoring materials	Saccharin, citronellal, synthetic vanillin	Food flavoring, cleaning product scents
Rubber processing chemicals	Thiuram, hexamethylene tetramine	Tires, adhesives
Plasticizers	Phosphoric acid, phthalic anhydride, and stearic acid	Rain coats, inflatable toys
Synthetic tanning agents	Naphthalene sulfonic acid condensates	Leather coats and shoes
Chemical warfare gases	Tear gas, phosgene	Military and law enforcement
Esters and/or amines of polyhydric alcohols and fatty and other acids	Allyl alcohol, diallyl maleate	Paints, electrical coatings
Cyclic crudes and intermediates	Benzene, toluene, mixed xylenes, naphthalene	Eyeglasses, foams
Cyclic dyes and organic pigments	Nitro dyes, organic paint pigments	Fabric and plastic coloring
Natural gum and wood chemicals	Methanol, acetic acid, rosin	Latex, adhesives

Sources: U.S. Department of Labor, 2001; American Chemistry Council, 2001.

On a volume basis, intermediate chemicals (chemicals that are subsequently processed into final products) represent the majority of the production in the organic chemicals industry. Figure 1 presents the annual production rate in 1998 of the ten most-produced intermediate chemicals in the U.S. The value of these shipments also are presented. These selected chemicals account for roughly 60% of the production volume of intermediates.

Figure 1: Annual Volume and Value of Common Organic Chemicals



Source: American Chemistry Council and Kline & Company, 1999.

II.B.2. Industry Size and Geographic Distribution

The organic chemicals industry accounted for approximately $80 billion in shipments in 2000, one fifth of the output of the entire chemical industry (U.S. Department of Commerce, 2000). As noted in Table 4, some facilities are quite large (greater than 500 employees). These facilities primarily produce bulk commodity chemicals such as those shown above in Figure 1. The industry is also characterized by a relatively high proportion of small facilities. These facilities predominantly manufacture specialty chemicals.

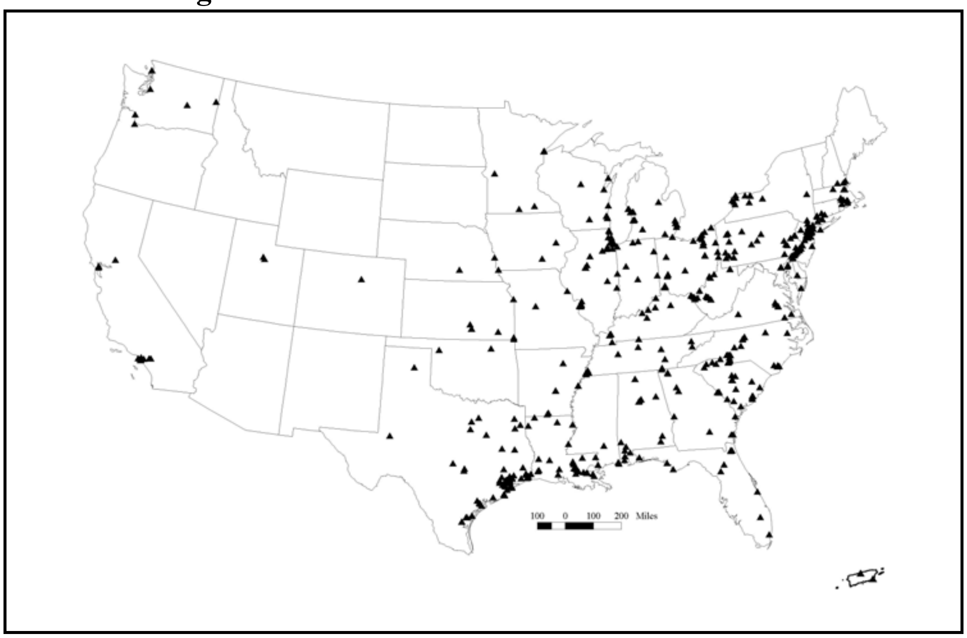
Table 4: Facility Size Distribution of Organic Chemical Facilities

Industry	Distribution of Facilities According to Number of Employees (% of Total in Parentheses)				
	1-19 Employees	20-99 Employees	100-499 Employees	>499 Employees	Total Facilities
Gum and wood chemicals (SIC 2861)	52 (74%)	10 (14%)	8 (11%)	0 (0%)	70 (100%)
Cyclic crudes and intermediates (SIC 2865)	75 (38%)	67 (34%)	51 (26%)	6 (3%)	199 (100%)
Industrial organic chemicals, not elsewhere classified (SIC 2869)	268 (36%)	254 (34%)	177 (24%)	44 (6%)	743 (100%)

Source: U.S. Department of Commerce, 1998.

Organic chemicals facilities generally are located in four areas of the United States. Gum and wood chemical production is found primarily in the southeast, near wood and pulp production facilities. Other organic chemicals facilities are predominantly located near the Gulf of Mexico, where many petroleum-based feedstocks are produced, and near downstream industrial users in the Northeast and Midwest.

Figure 2: Geographic Distribution of U.S. Organic Chemical Manufacturing Facilities



There are no organic chemical facilities in Alaska or Hawaii.
Source: U.S. EPA, Toxics Release Inventory Database, 1999.

II.B.3. Economic Trends

The United States has the largest organic chemicals industry in the world and is a net exporter of organic chemicals. However, many of the chemicals produced by the industry are commodities. As a result, the industry faces significant competition due to increased capacity in Asia, the Middle East, and Latin America. Difficulties between 1998 and 2001 included reduced shipments to Asia because of its slowed economy, worldwide overcapacity, and higher raw material and fuel costs due to high oil prices (U.S. Department of Commerce, 2000).

Several trends are occurring within the industry to account for these and other changes. A considerable amount of consolidation is occurring. Across the chemical industry as a whole, there was approximately $45 billion in mergers and acquisitions in 1999 (U.S. Department of Commerce, 2000). Furthermore, many chemical companies are repositioning themselves in fundamental ways. Companies such as ICI, Clariant, and Ciba now focus on specialty chemicals. Others, including Exxon, BP, and Shell, now produce basic chemicals almost exclusively. Finally, some former chemical companies, such as Monsanto, Hoechst, and Novartis, exited the organic chemicals industry to specialize in life sciences (Speed, 2001). Table 5 lists the top 10 companies in the United States in 2001 according to their sales of chemicals.

In the longer term, anticipated sustained growth in downstream industries such as agricultural chemicals (fertilizers and pesticides) and pharmaceuticals are expected to provide growth opportunities for the organic chemicals industry (Speed, 2001).

Table 5: Top 20 U.S. Chemical Producers in 2001

Rank	Company	2001 Chemical Sales[a] (millions of dollars)
1	Dow Chemical	27,805
2	DuPont	26,787
3	ExxonMobil	15,943
4	Huntsman Corp.	8,500
5	General Electric	7,069
6	BASF	6,852
7	Chevron Phillips	6,010
8	PPG Industries	5,933
9	Equistar Chemicals	5,909
10	Shell Oil	5,524
11	Air Products	5,467
12	Eastman Chemical	5,384
13	BP	5,300
14	Praxair	5,158
15	Rohm and Haas	4,917
16	Atofina	4,380
17	Monsanto	3,755
18	Honeywell	3,313
19	Lyondell Chemical	3,226
20	Nova Chemicals	3,194

[a] Represents sales from chemical segment of each company; organic chemicals may only be a portion of these sales.
Source: "Annual Survey: Top 75 Chemical Producers." *Chemical & Engineering News*, Volume 80, Number 19 (May 13, 2002); 21-25.

III. INDUSTRIAL PROCESS DESCRIPTION

This section describes the major industrial processes within the organic chemical industry, including the materials and equipment used, and the processes employed. The section is designed for those interested in gaining a general understanding of the industry, and for those interested in the inter-relationship between the industrial process and the topics described in subsequent sections of this profile -- pollutant outputs, pollution prevention opportunities, and Federal regulations. This section does not attempt to replicate published engineering information that is available for this industry. Refer to Section IX for a list of reference documents that are available.

This section specifically contains a description of commonly used production processes, associated raw materials, the by-products produced or released, and the materials either recycled or transferred off-site. This discussion, coupled with schematic drawings of the identified processes, provides a concise description of where wastes may be produced in the process. This section also describes the potential fate (via air, water, and soil pathways) of these waste products.

III.A. Industrial Processes in the Organic Chemicals Industry

Although the organic chemicals industry manufactures thousands of chemicals, there are basic principles that are common to most production processes. This section provides a brief overview of the processes, describes common chemical reactions, and discusses four chemicals that are particularly important building blocks for organic chemical products.

III.A.1. Chemical Manufacturing Processes

As described in Section II, the organic chemicals industry requires raw materials from upstream industries, such as petroleum refining, and sells its products either as finished materials or as intermediates for further processing by other manufacturers. Assuming that raw materials are received in sufficient purity, the two major steps in chemical manufacturing are 1) the chemical reaction and 2) the purification of reaction products.

Chemical Reaction Processes

The primary types of chemical reactions are *batch* and *continuous*. In *batch reactions*, the reactant chemicals are added to the reaction vessel at the same time and the products are emptied completely when the reaction is completed. The reactors are made of stainless steel or glass-lined carbon steel and range in size from 50 to several thousand gallons (U.S. EPA, 1993). Batch reactors, also called stirred tank reactors or autoclaves, have an agitator mechanism to mix the reactants, an insulating jacket, and the appropriate pipes and valves to control the reaction conditions (U.S. EPA, 1993; Kroschwitz, 1986).

Batch processes generally are used for smaller scale and experimental processes. One advantage is that batch equipment can be adapted to multiple uses – an important issue for facilities producing many specialty chemicals. Also, these processes are easier to operate, maintain, and repair. In general, facilities producing less than four million pounds of a particular product per year use a batch process (Hocking, 1998).

An important subcategory of the batch process is *toll manufacturing*. Many organic chemicals require multi-step manufacturing processes. These steps often call for precise operating conditions, which in turn demand specialized equipment and trained employees. In a tolling operation, a company outsources one or more steps in the manufacturing process to a contractor, who then sends the product to yet another contractor to complete the production process. Toll manufacturing is highly useful from an engineering standpoint, but this arrangement can also be used for economic reasons to utilize excess production capacity.

Continuous processes occur either in a tank (a "continuous stirred tank reactor") or in a pipe (a "pipe reactor"). In this case, the reactants are added and products are removed at a constant rate from the reactor, so that the volume of reacting material in the vessel remains constant. A continuous stirred tank reactor is similar to the batch reactor described above. A pipe reactor typically is a piece of tubing arranged in a coil or helix shape that is jacketed in a heat transfer fluid. Reactants enter one end of the pipe, and the materials mix under the turbulent flow and react as they pass through the system. Pipe reactors are well suited for reactants that do not mix well, because the turbulence in the pipes causes all materials to mix thoroughly (Hocking, 1998).

Continuous processes require a substantial amount of automation and capital expenditures, and the equipment generally must be dedicated to a single product. As a result, this type of process is used primarily for large scale operations, such as those producing greater than 20 million pounds per year of a particular chemical (Hocking, 1998). For facilities producing between 4 and 20 million pounds of a chemical per year, the choice of a batch or continuous process depends on the particular chemical and other site-specific considerations.

In some cases, a hybrid reaction process, called a semi-batch reactor, is needed. This is commonly used when the reaction is very fast and potentially dangerous. One reactant is placed in the vessel at the beginning of the reaction (like in a batch process) and the other reactant(s) is added gradually (Hocking, 1998).

Product Separation

Reaction products rarely are obtained in a pure form from a reaction. Often there are byproducts and unreacted inputs. Therefore, the desired product must be isolated and purified in order to be used by customers or downstream manufacturers. Common separation methods include filtration, distillation, and extraction. Depending on the particular mixture and the desired purity, multiple separation methods can be used.

Filtration
Filtration is a process that separates solids from liquids. A slurry, or mixture of liquid and suspended particles, is passed through a porous barrier (filter) that traps the solids and allows the liquid to pass through. The liquid typically is passed through the filter via gravity. An alternative form of filtration is *centrifugation*, in which the slurry is placed in a porous basket that is spun rapidly. The outward force pushes the liquid through the filter or mesh on the sides of the basket where the fluid is reclaimed.

Distillation
Distillation is a process that separates liquids that have differing boiling points. A mixture of liquids is heated to the boiling point of the most volatile compound (i.e., the compound with the lowest boiling point). That compound becomes gaseous and then is condensed back to a liquid form in an attached vessel. Additional compounds can be isolated from the mixture by increasing the temperature incrementally to the appropriate boiling point. It should be noted that materials existing as gases at room temperature can be separated via distillation when they are refrigerated to a liquid form and slowly warmed to their boiling points.

Extraction
Organic compounds each have different solubility rates in fluids such as water or organic solvents. In an extraction, a mixture is placed in a fluid in which the desired product is insoluble but the undesired materials are soluble. The result is that the desired material is in a separate phase from the solvent and contaminants and can be removed (Buonicore and Davis, 1992).

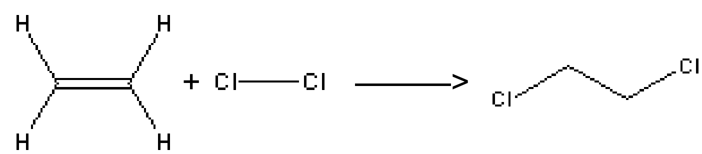
III.A.2. Common Chemical Reactions

The following section presents some of the chemical reactions that are used to produce the most significant products of the organic chemicals industry, such as those listed in Figure 1 in Section II. There are illustrations of each type of reaction. Note that the illustrations follow the chemistry standard practice of implying that a carbon atom is found wherever lines meet.

Details of the reactions were obtained form *Organic Chemistry by* Vollhardt and Schore, and the equation illustrations were obtained from the internet site http://products.cambridgesoft.com/ChemFinder.cfm.

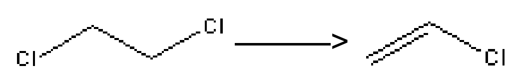
Halogenation

Halogenation is a process of adding a halogen atom on an organic compound. (Halogen is the collective name for fluorine, chlorine, bromine, and iodine.) This is an important step in making chlorinated solvents such as ethylene dichloride. The following equation shows a simplified version of the halogenation of ethylene to form ethylene dichloride. This particular reaction generally is conducted with an iron chloride catalyst. (A catalyst is material that facilitates a reaction but is not actually consumed in the process).



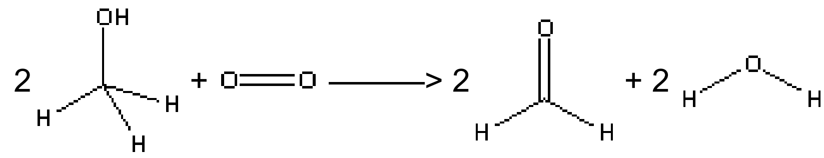
Pyrolysis

Pyrolysis is a process of breaking down a large compound into smaller components by heating it (in the absence of oxygen) and exposing it to a catalyst. This process is also referred to as *cracking*. Vinyl chloride is produced in this way by pyrolizing ethylene dichloride. Because pyrolysis can result in a variety of products, the catalyst and temperature must be carefully selected and controlled in order to maximize the yield of the desired product. The following equation shows the formation of vinyl chloride in the presence of heat and a catalyst.



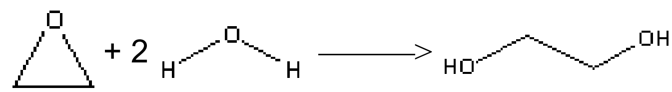
Oxidation

In the context of organic chemistry, oxidation generally means the addition of an electron-donating atom (such as oxygen) and/or the removal of hydrogen to a compound. For example, formaldehyde is formed by removing two hydrogen atoms from methanol, as shown in the following equation. Oxygen and a metal catalyst, such as silver, typically are used in the reaction.



Hydrolysis

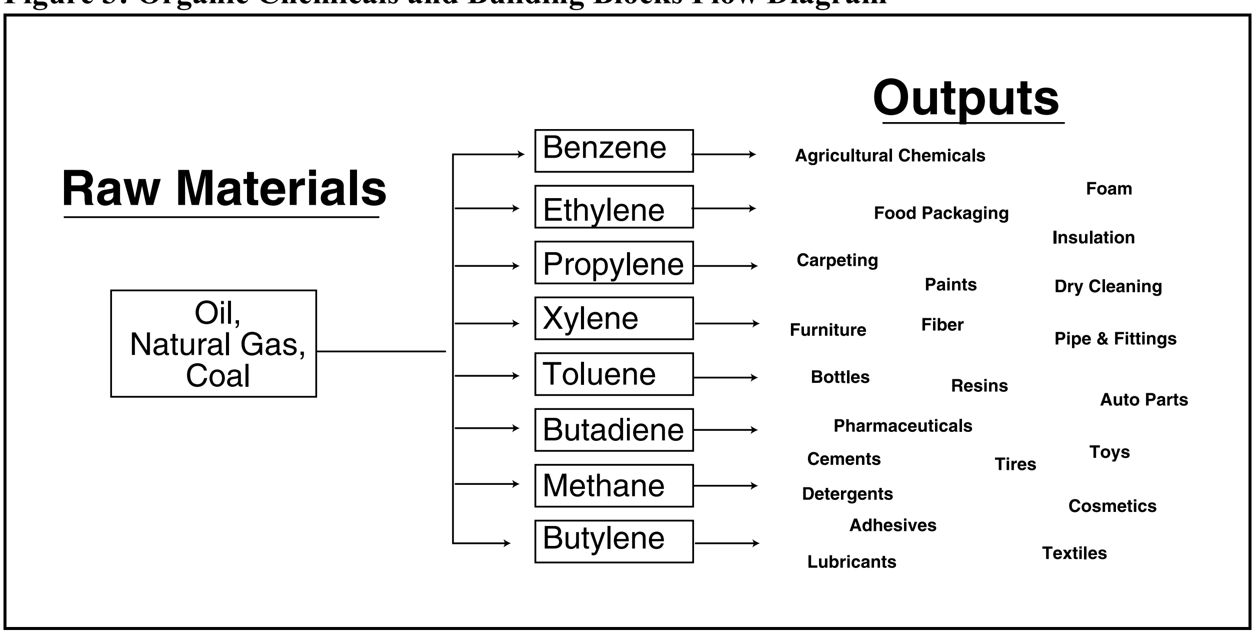
Hydrolysis involves the addition or substitution of water (H_2O) into a compound. This process is used in the manufacturing of ethylene glycol, the main component of antifreeze. The following equation shows how ethylene oxide is hydrolized to form ethylene glycol.



III.A.3. Common Organic Chemical Production Chains

Most of the products of the organic chemicals industry are derived from just a handful of *feedstocks*, or raw materials. Figure 3 demonstrates this conceptually; a small number of chemicals derived from materials such as fossil fuels are then processed into the wide range of intermediate and finished products used in the economy.

Figure 3: Organic Chemicals and Building Blocks Flow Diagram



The rest of this section presents the reactions of three high-volume chemicals (ethylene, propylene, and benzene) chosen to illustrate the use of typical chemical feedstocks. The three chemicals are all primary building blocks and their reaction products are used to produce still other chemicals. The flowcharts below (Figures 4-6) illustrate some of the common intermediates and final products associated with each chemical.

The chemicals described below illustrate several key points. First, primary building blocks are typically used in more reactions than the building blocks further down the chain. Second, most feedstocks can participate in more than one reaction and third, there is typically more than one reaction route to an end-product. The end-products of all of these chemicals can be used in numerous commercial applications; *Riegel's Handbook of Industrial Chemistry,* listed in the reference section, describes many uses.

Ethylene

The major uses for ethylene are in the synthesis of polymers (polyethylene) and in ethylene dichloride, a precursor to vinyl chloride. Other important products are ethylene oxide (a precursor to ethylene glycol) and ethylbenzene (a precursor to styrene). While ethylene itself is not generally considered a health threat, several of its derivatives, such as ethylene oxide and vinyl chloride, have been shown to cause cancer. The distribution of uses is shown in Table 6.

The manufacturing processes that use ethylene as a feedstock are summarized in the table below along with reaction conditions and components. Ethylene dichloride, ethylbenzene, and ethylene oxide (products of ethylene reactions) are all among the top 50 high production volume organic chemicals in the United States (*Chemical and Engineering News*).

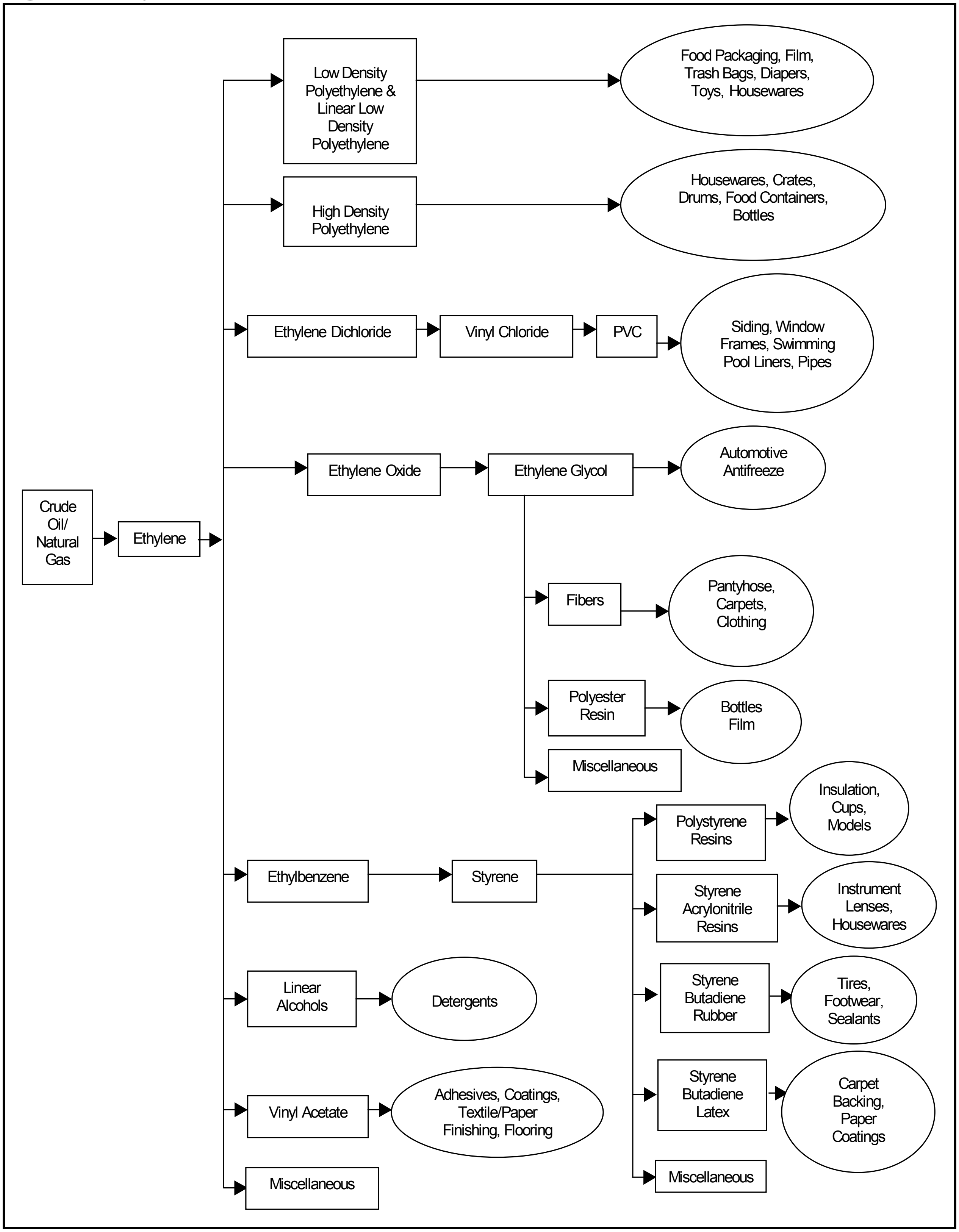
Table 6: Distribution of Uses for Ethylene

Product	Percent of Ethylene Use
Polyethylene	54
Ethylene dichloride	16
Ethylene oxide-glycol	13
Ethylbenzene-styrene	7
Linear olefins-alcohol	3
Vinyl acetate	2
Ethanol	1
Other	4

Source: *Kirk-Othmer Encyclopedia of Chemical Technology*.

Figure 4 presents a flowchart of the intermediates produced from ethylene and examples of the major finished products. Many of the products are plastics derived from polyethylene.

Figure 4: Ethylene Products



Source: American Chemistry Council, 2001.

Propylene

Over half of the U.S. propylene supplies are used in the production of chemicals. The primary products are polypropylene, acrylonitrile, propylene oxide, and isopropyl alcohol. Of these, propylene, acrylonitrile and propylene oxide are among the top fifty high-volume chemicals produced in the United States. Acrylonitrile and propylene oxide have both been shown to cause cancer, while propylene itself is not generally considered a health threat. Table 7 shows the use distribution of propylene.

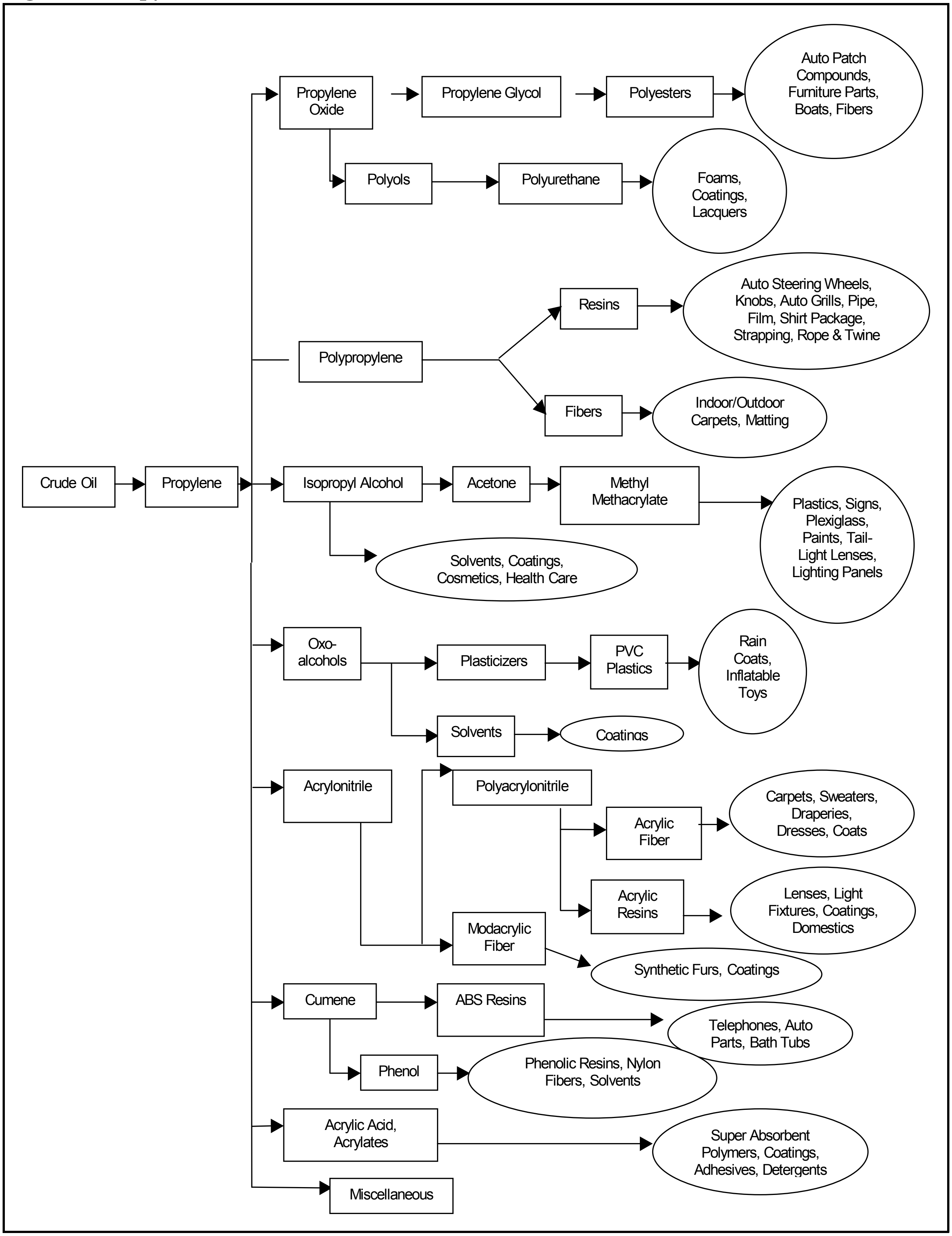
Table 7: Distribution of Propylene Use

Product	Percent of Propylene Use
Polypropylene	36
Acrylonitrile	16
Propylene oxide	11
Cumene	9
Butyraldehydes	7
Oligomers	6
Isopropyl alcohol	6
Other	9

Source: Szmant.

Figure 5 shows the major intermediates and finished products associated with propylene.

Figure 5: Propylene Products



Source: American Chemistry Council, 2001.

Benzene

Benzene is an important intermediate in the manufacture of industrial chemicals. Over 95 percent of U.S. consumption of benzene is for the preparation of ethylbenzene, cumene, cyclohexane, nitrobenzene, and various chlorobenzenes as shown in Table 8. Benzene is considered a human carcinogen by EPA.

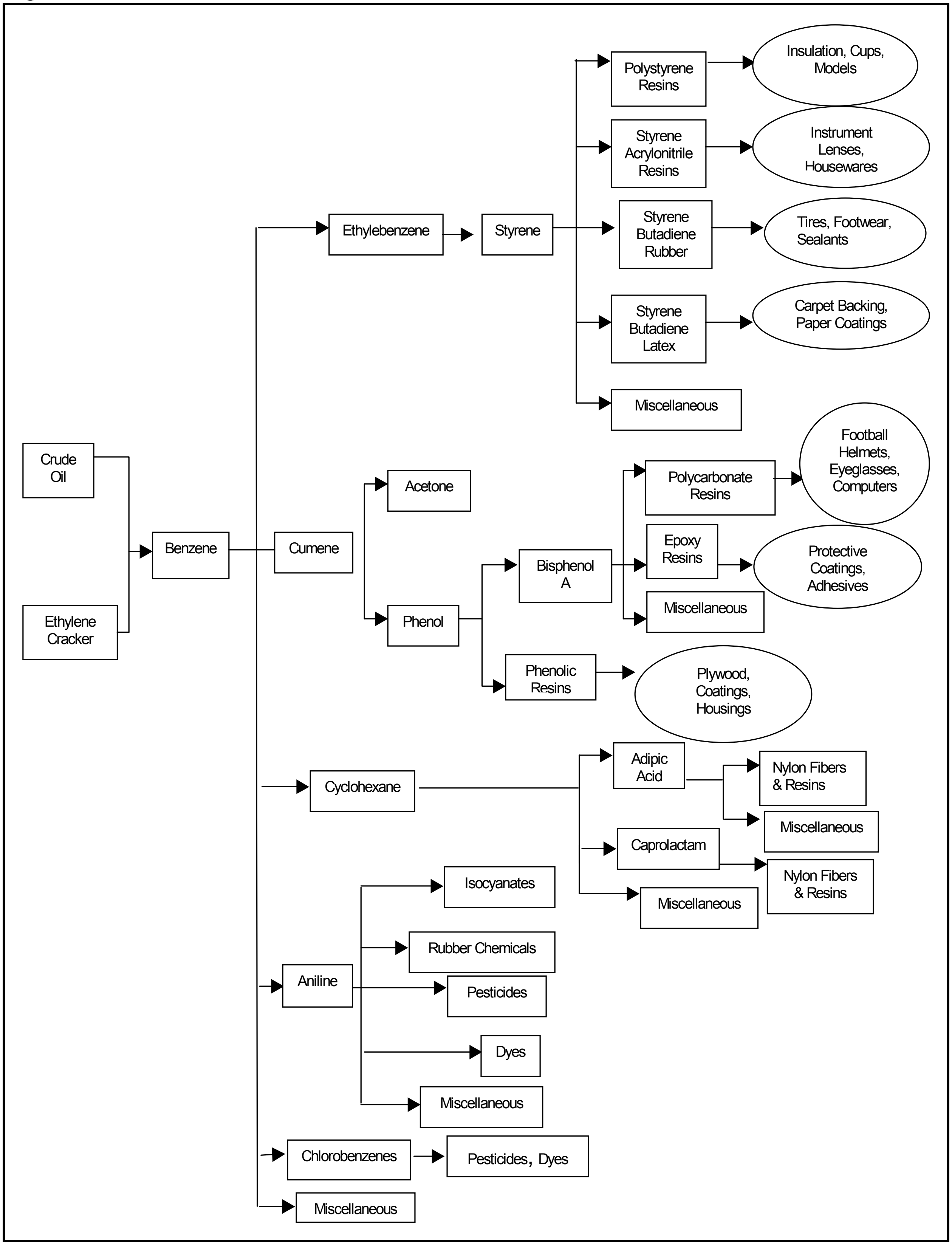
Table 8: Distribution of Benzene Use

Product	Percent of Benzene Use
Ethylbenzene	52
Cumene	22
Cyclohexane	14
Nitrobenzene	5
Chlorobenzenes	2
Linear detergent alkylate	2
Other	3

Source: *Kirk-Othmer Encyclopedia of Chemical Technology*.

Figure 6 summarizes the primary benzene intermediates and products.

Figure 6: Benzene Products



Source: American Chemistry Council, 2001.

III.B. Raw Material Inputs and Pollution Outputs

Industrial organic chemical manufacturers use and generate both large numbers and quantities of chemicals. The industry releases chemicals to all media including air (through both fugitive and direct emissions), water (direct discharge and runoff) and land. The types of pollutants a single facility will release depend on the feedstocks, processes, equipment in use and maintenance practices. These can vary from hour to hour and can also vary with the part of the process that is underway. For example, for batch reactions in a closed vessel, the chemicals are more likely to be emitted at the beginning and end of a reaction step (associated with vessel loading and product transfer operations), than during the reaction. The potential sources of pollutant outputs by media are shown below in Table 9.

Table 9: Potential Releases During Organic Chemical Manufacturing

Media	Potential Sources of Emissions
Air	Point source emissions: stack, vent (e.g. laboratory hood, distillation unit, reactor, storage tank vent), material loading/unloading operations (including rail cars, tank trucks, and marine vessels) Fugitive emissions: pumps, valves, flanges, sample collection, mechanical seals, relief devices, tanks Secondary emissions: waste and wastewater treatment units, cooling tower, process sewer, sump, spill/leak areas
Liquid wastes (Organic or Aqueous)	Equipment wash solvent/water, lab samples, surplus chemicals, product washes/purifications, seal flushes, scrubber blowdown, cooling water, steam jets, vacuum pumps, leaks, spills, spent/used solvents, housekeeping (pad washdown), waste oils/lubricants from maintenance
Solid Wastes	Spent catalysts, spent filters, sludges, wastewater treatment biological sludge, contaminated soil, old equipment/insulation, packaging material, reaction by-products, spent carbon/resins, drying aids
Ground Water Contamination	Unlined ditches, process trenches, sumps, pumps/valves/fittings, wastewater treatment ponds, product storage areas, tanks and tank farms, aboveground and underground piping, loading/unloading areas/racks, manufacturing maintenance facilities

Source: Chemical Manufacturers Association, 1993.