To the Graduate Student Council:

I am submitting herewith a dissertation written by Susan Marie Sharp entitled "Impact Assessment for the Life Cycle Assessment of a Manufactured Product Using a Chemical Ranking and Scoring System." I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Life Sciences.

Walter Farkas, Major Professor

We have read this dissertation
and recommend its acceptance:

Accepted for the Council:

Associate Vice Chancellor and
Dean of the Graduate School

IMPACT ASSESSMENT FOR THE LIFE CYCLE ASSESSMENT OF A MANUFACTUREDPRODUCT USING A CHEMICAL RANKING AND SCORING SYSTEM

A Thesis
Presented for the
Master of Science
Degree
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Susan Marie Sharp
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DEDICATION

This thesis is dedicated to my family

Richard, Jessica, and Martina Ward

who gave me their love and encouragement.

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ABSTRACT

In this study an algorithm for a chemical ranking and scoring system is developed and applied to the impact assessment phase of a product life cycle assessment. The algorithm is a modification of a previous model developed by researchers at the University of Tennessee and includes the toxicological endpoint of the no observable adverse effect level (NOAEL). The chemical ranking and scoring system is used to assign a numerical value which is a measure of the potential hazard associated with a specific chemical release from a manufacturing process. These hazard values are calculated based on physical and chemical properties, the quantity released, and standard toxicological endpoints. The summation of these hazard values are used to compare information from a life cycle assessment for two identified phases of the manufacture of a plastic material to determine the phase which has the greatest potential for adverse environmental effects. From the algorithm in this study the first phase of production of a high density polyethylene plastic is determined to be 9159 and the second phase of production is determined to be 5418. Therefore, the first production phase is identified as having a greater potential environmental impact than the second production phase. These values are to be used for relative ranking comparison only and cannot be divided into each other to make a mathematical statement about degree of hazard.

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ABBREVIATIONS

BCF	- Bioconcentration Factor
BOD	- Biological Oxygen Demand half-life
Carcin	- Carcinogenicity
CRS	- Chemical Ranking and Scoring
EM	- Exposure Multiplier
FishLC50	- Lethal Concentration in water in mg/l for 50% of test subjects (fish)
FishNOEL	- No Observed Effect Level in water in mg/l for test subjects (fish)
HDPE	- High Density Polyethylene
HEAST	- Health Effects Assessment Summary Table of the U.S. EPA
HV	- Hazard Value
HYD	- Hydrolysis half-life
IARC	- International Agency for Research on Cancer
Inh	- Inhalation
IUCLID	- International Uniform Chemical Information Database of the European Chemical Bureau
LCA	- Life Cycle Assessment
LC50	- Lethal Concentration in air for 50% of test subjects (rodents) in inhalation in ppm
LD50	- Lethal Dose ingested for 50% of test subjects (rodents) in oral mg/kg-day

LOAEL	- Least Observable Adverse Effect Level for test subjects (rodents) in oral mg/kg-day or inhalation mg/m^3
NOAEL	- No Observable Adverse Effect Level for test subjects (rodents) in oral mg/kg-day or inhalation mg/m^3
NOEL	- No Observable Effect Level
Orl	- Oral
QSAR	- Quantitative Structure Activity Relationship
RfD	- Reference Dose in oral mg/kg-day
RfC	- Reference Concentration in inhalation mg/m^3
SETAC	- Society of Environmental Toxicology and Chemistry
U.S. EPA	- United States Environmental Protection Agency

INTRODUCTION

Releases of toxic substances to the air, water, and land occur frequently as a result of manufacturing processes. Assessment of the risks to the human population and the environment from industrial releases is an important concern for the industry releasing the chemicals and for the general public who could potentially be exposed to the waste. The Life Cycle Assessment (LCA) of a product is a "cradle-to-grave" analytic tool which enables comparisons of the energy consumption, the resource use, and the environmental impacts of manufacturing a product. Currently the impact assessment aspect of the Life Cycle Assessment is not well developed or standardized (Davis, Personal communication 1995). Chemical ranking and scoring systems (CRS) are risk assessment algorithms which evaluate the relative risk of toxic chemicals based on their toxicity, environmental persistence, and exposure quantities. The purpose of this thesis is to apply a chemical ranking and scoring system to an impact assessment to determine the relative impact of environmental toxicants released in two phases of the manufacturing of a plastic product.

CHAPTER I

LIFE CYCLE ASSESSMENT

Life Cycle Assessment (LCA) involves taking an inventory of the chemicals released and making an assessment of the environmental impacts of those chemicals. LCA enables comparisons to be made between the environmental impacts of different products or between different manufacturing processes for the same product; therefore, it is an important and useful tool for pollution prevention and design decision making. Endpoints from toxicological testing of chemicals provide an indication of the potential hazard from exposure to that chemical. Although toxicological endpoints have been considered in LCA impact assessments, the relative ranking of the chemicals released has not been used to compare the potential risks of manufacturing processes.

Data from the manufacture of high density polyethylene plastic are analyzed by a chemical ranking and scoring system (CRS). The source for these data are personal communication with Gary Davis at the Center for Clean Products and Clean Technologies (CCPCT) at the University of Tennessee Knoxville. The manufacturing process for HDPE is broken down into two production phases. The first phase is the production of the intermediate plastic olefin and is referred to as the Olefin phase. The second phase is the manufacturing step from olefin to the final HDPE product which is referred to as the HDPE phase. The chemicals released in the Olefin phase of production to air, water, and land in pounds (lbs) of chemical per pound of final HDPE manufactured are listed in

Table 1. The chemicals released during the HDPE phase of production to air, water, and land are listed in Table 2.

An overall hazard value is calculated for chemicals released during the two production phases in the manufacturing the final HDPE plastic. The sums of the total hazard values of the Olefin phase and the HDPE phase are compared to each other in order to make a relative statement about which phase of the production process might involve the most environmental risk. This information is then used to identify the phase in which the greatest improvement could be made when a company tries to reduce adverse environmental effects.

This thesis applies a modified version of the chemical ranking and scoring system developed by Gary Davis, et al. at the University of Tennessee Center for Clean Products and Clean Technologies to the toxic emissions from a Life Cycle Assessment of the manufacturing process of a HDPE plastic material. The modifications of this chemical ranking and scoring system involve the omission of one endpoint worth a total of 5 points which was based on the number of articles written about the chemical which appeared in the ROADMAPS database. This hazard value (HV) was designated as HV_{other} in the CCPCT report (Davis et al., 1994). An additional hazard value score worth 5 points for the toxicology endpoint of the oral No Observable Adverse Effect Level (NOAEL) is developed and substituted in this presentation of the modified version. The inhalation NOAEL is used to determine a hazard value score if the oral NOAEL is not available.

Table 1. Olefin Air, Water, and Land Releases		
CHEMICAL	EMISSION MEDIA	LBS OF CHEMICAL PER LB OF PRODUCT
1,3-Butadiene	air	2.47E-05
1,3-Butadiene	land	2.73E-09
1,3-Butadiene	water	8.33E-10
Acetone	air	5.26E-07
Ammonia	air	6.05E-08
Ammonia	water	1.02E-07
Ammonium Sulfate	water	2.00E-05
Asbestos (fri)	land	3.17E-05
Benzene	air	5.37E-05
Benzene	land	1.89E-06
Benzene	water	4.03E-07
Biphenyl	air	8.76E-08
Biphenyl	water	3.32E-12
Carbon Disulfide	air	5.83E-07
Carbon Disulfide	land	6.09E-09
Chromium Compounds	land	8.15E-09
Chromium Compounds	water	8.70E-09
Copper Compounds	land	2.15E-10
Copper Compounds	water	2.79E-08
Cumene	air	1.74E-07
Cumene	water	2.42E-11
Cyclohexane	air	1.57E-06
Epichlorohydrin	air	9.21E-08
Ethylbenzene	air	6.08E-06
Ethylbenzene	land	2.10E-07
Ethylbenzene	water	1.16E-07
Ethylene	air	2.77E-04
Ethylene	water	7.07E-09
Ethylene Glycol	air	1.42E-07
Ethylene Glycol	land	1.04E-09
Ethylene Glycol	water	5.95E-09
Lead Compounds	land	6.14E-11
m-Xylene	air	7.38E-07
m-Xylene	water	3.07E-11

Source: Gary Davis. Director of the Center for Clean Products and Clean Technologies in the Energy and Environment Resource Center at the University of Tennessee, Knoxville.

Table 1. (continued)		
CHEMICAL	**EMISSION MEDIA**	**LBS OF CHEMICAL PER LB OF PRODUCT**
Manganese Compounds	water	6.29E-09
Methanol	air	2.26E-05
Methanol	water	3.06E-09
Methyl Ethyl Ketone	air	1.52E-08
Methyl Ethyl Ketone	land	3.00E-07
Methyl Isobutyl Ketone	air	1.11E-07
Methyl Isobutyl Ketone	land	2.62E-08
Naphthalene	air	2.23E-05
Naphthalene	land	4.93E-07
Naphthalene	water	3.52E-08
Nickel Compounds	land	3.70E-07
o-Xylene	air	3.45E-07
p-Xylene	air	3.54E-07
Phenol	air	2.78E-08
Phenol	water	3.00E-04
Phosphoric Acid	air	3.48E-08
Propylene	air	1.98E-04
Propylene	water	5.25E-08
Styrene	air	2.12E-06
Styrene	land	7.00E-08
Styrene	water	6.99E-09
Tetrachloroethylene	air	1.26E-10
Toluene	air	1.63E-05
Toluene	land	2.89E-06
Toluene	water	2.99E-04
Trichloroethylene	air	1.26E-10
Vinyl Acetate	air	3.39E-08
Xylene (mix)	land	4.88E-06
Xylene (mix)	water	5.34E-08
Xylene(mixed)	air	2.45E-06
Zinc Compounds	land	5.00E-08
Zinc Compounds	water	2.83E-08

Source: Gary Davis. Director of the Center for Clean Products and Clean Technologies in the Energy and Environment Resource Center at the University of Tennessee, Knoxville.

Table 2. HDPE Air, Water, and Land Releases		
CHEMICAL	**EMISSION SOURCE**	**LBS OF CHEMICAL PER LB OF PRODUCT**
Acetone	air	2.02E-09
Ammonia	water	1.54E-08
Asbestos (fri)	land	2.62E-07
Carbon Disulfide	air	7.27E-08
Chromium Compounds	air	1.02E-07
Chromium Compounds	water	2.13E-06
Chromium Compounds	land	5.44E-07
Copper Compounds	water	7.88E-07
Ethylene	air	2.24E-04
Lead Compounds	water	1.08E-07
Manganese Compounds	water	2.70E-06
Methanol	air	1.85E-06
Nickel Compounds	water	1.08E-07
Phosphoric Acid	air	6.59E-10
Propylene	air	7.35E-07
Propylene Oxide	air	1.33E-06
Tetrhydorfuran	air	1.33E-06
Toluene	air	1.08E-06
Xylene (mixed)	air	1.45E-08
Zinc Compounds	water	3.76E-06

Source: Gary Davis. Director of the Center for Clean Products and Clean Technologies in the Energy and Environment Resource Center at the University of Tennessee, Knoxville.

Definition of Life Cycle Assessment

LCA is a "cradle-to-grave" analytic tool used to identify the environmental consequences of a manufacturing process or a product through its entire lifetime. Energy and resource inputs and outputs are considered for the entire life cycle stages of a product including raw material acquisition, manufacturing, transportation, use and maintenance, and disposal or recycling (SETAC, 1992).

LCA consists of three components involving the analysis of inventory, the impact assessment, and the improvement assessment. The Society of Environmental Toxicology and Chemistry (SETAC) developed definitions for these three components. The inventory is primarily a list consisting of "materials and energy used and environmental releases arising from all stages in the life of a product or process, from raw material acquisition to ultimate disposal" (SETAC, 1992). The impact assessment involves "examining potential and actual environmental and human health effects related to the use of resources (energy and materials) and environmental releases" (SETAC, 1992). The improvement assessment evaluates "the changes needed to bring about environmental improvements in the product or process" (SETAC, 1992).

Information derived from an LCA about the environmental impacts of all stages involved in making a product has many potential uses. Fred Moavenadeh outlined five basic approaches to controlling waste at the source in his book *Global Construction and the Environment: Strategies and Opportunities* (Moavenadeh, 1994). These approaches are to change raw materials, to change production technology and equipment, to improve

production operations and procedures, to recycle waste within the plant, and to redesign or reformulate end products. LCA would provide useful information for decision makers trying to reduce waste at the source using any of these five approaches.

Companies wanting to compete successfully in the current competitive marketplace must be able to respond to customer demands for environmentally preferable products, to comply with costly and complicated environmental regulations, to prevent pollution, and to minimize the need for expensive environmental remediation. Industries able to design products which are of high quality and which can be demonstrated to be environmentally cleaner than similar products of other companies will have a competitive advantage. Current strategies used by the United States Environmental Protection Agency (U.S. EPA) to reduce pollution focus on voluntary efforts at pollution prevention (Elliot, 1993). Many companies are directing their environmental efforts to pollution prevention through better and more efficient management of the manufacturing process and product design (Parker, 1993). Life Cycle Assessments of the impacts of comparable product designs or a manufacturing processes is one way to accomplish pollution prevention (Tolle, 1994).

LCA could be useful for promotion of Sustainable Development. Joseph Fiksel defines Sustainable Development as economic progress that meets the needs of the present without compromising the ability of future generations to meet their own needs (Fiskel, 1993). The Earth Summit in Rio de Janeiro, Brazil in 1992 recognized the concept that industrial growth and environmental quality are both necessary and need not

be mutually exclusive (Fiksel, 1993). Reducing the quantities of toxic materials produced in the manufacturing process is a cost effective pollution control strategy of the EPA's Design for the Environment (DFE) program. The design stage is the most critical time to consider the environmental impacts of a product and to make waste minimization decisions (Parker, 1993). LCA is useful for decision making during the manufacturing process because the contributions of individual steps in product development can be evaluated for their impact. This evaluation enables the company to make internal improvement in the product design process thereby reducing pollution (Vigon, 1993).

Consumers interested in purchasing products with the least impact on the environment would benefit from having information from the LCAs of comparable products. Companies who evaluate the LCAs for their own products and for those of their competition could increase sales to motivated consumers by advertising the environmental advantage of their products on the label (Davis, 1993).

A final use for LCA information is for the identification of a phase of the production process which potentially contains the most adverse environmental impact. Identification of the production phase which has the most harmful environmental effect is useful to a company trying to reduce the overall pollution released in the manufacturing process. The inventories of the various production phases are analyzed separately and then are compared to each other. It is this final application of LCA for identifying the most harmful phase of a production process which is presented in this thesis.

Impact Assessment Strategies

Various impact assessment strategies were studied and are presented here to illustrate the limits of only discussing LCAs qualitatively while not trying to quantify the adverse effects of the pollution.. Classification and stressor category selection is a major emphasis of the LCA strategies published in the literature. Impact characterization is not usually presented in papers and reports on LCA. The CRS approach to LCA impact characterization is unique and could prove useful for determining the impacts of harmful chemical releases. Most of the impact assessment studies presented here only classify the environmental problems due to industrial releases. Only one study presented a protocol for how an impact assessment characterization for chemicals releases could be done (Centre of Environmental Science, 1992).

The Society of Environmental Toxicologists and Chemists (SETAC) published an LCA framework based on a March 1992 workshop (SETAC, 1992). The impact classifications and categorizations are discussed in general terms, but there are no strategies presented for quantifying or calculating an impact. The classes are defined but specific examples are not given in the report or the appendix. The stressor categories are presented as ecological stressors including climate change gases, ozone depletors, toxicants, acidification precursors, photochemical oxidants, and nutrients; human health impacts including acute and chronic effects; resource depletion of both renewable and non-renewable resources; and social welfare effects (SETAC, 1992).

The National Reuse of Waste Research Programme in the Netherlands published a

report called "Environmental Life Cycle Assessment of Products: Backgrounds and Guide - October 1992" (Centre of Environmental Science, 1992). This report presents methods to calculate values, called "potentials", for specific chemicals which can be multiplied by exposures to calculate quantities which can be compared to each other. For toxic chemicals, the potential values are based on European regulatory values for safe daily exposures. American regulatory values are not recommended for use as risk assessment toxicology endpoints because they are usually general values which are not based on extensive testing of the particular chemical but are frequently based on test results from similar chemicals (Swanson, Personal communication 1995). Comparing Permissible Exposure Levels (PEL) in the *Sax's Dangerous Properties of Industrial Materials* one finds only a few values such as inhalation at 100 ppm, 200 ppm, or 1000 ppm; but there are not usually values of greater precision (Lewis, 1992). The general method for calculating the potentials is presented in the background report and specific examples are presented in the appendix of that report. Stressor categories are numerous and include the following: depletion of abiotic and biotic resources, pollution effects from greenhouse gases, depletion of the ozone layer, human toxicity, aquatic and terrestrial ecotoxicity, photochemical oxidant formation, acidification, nutrification, radiation, waste heat, noise, odor, working conditions; and damage to ecosystems, landscapes, and human victims (both directly and indirectly). This report presents the greatest number of stressor categories of any of the reports considered, however many of the categories are primarily aesthetic rather than health or pollution related.

The Phosphate Report is a scoring system for pollutants by Bob Wilson and Bryn Jones (Wilson et al., 1994). This report relies on the Delphi Technique of expert opinion for evaluation of environmental impacts. In the Delphi Technique a panel of experts independently answers a questionnaire. Then they are asked to look at the responses of the other experts and to decide if they want to keep their original response or if they want to change it closer to or further from the average response. In this assessment the impacts are never assigned to impact classification categories. A weighted score is assigned to each of the chemical outputs based on expert opinion and not on toxicological endpoints.

These impact reports are of limited use to risk assessors. While they do a good job of classifying the impacts and addressing the important social issues, they do not present ways to quantify the adverse effects of pollution.

CHAPTER II

CHEMICAL RANKING AND SCORING SYSTEMS

Chemical ranking and scoring systems are risk assessment tools for comparing the relative risks of exposure to different chemicals based on consideration of impacts on human health, the terrestrial environment, and the aquatic environment. Toxicological endpoints and the exposure properties of persistence and bioconcentration are used in an algorithm to quantify a value for the potential hazard for each chemical. These hazard values are compared and the chemicals considered are ranked from highest to lowest risk relative to each other. SETAC sponsored a Chemical Ranking and Scoring Workshop in Destin, Florida in February of 1995 in order to develop a consensus framework to promote consistency in the development and the application of CRS (SETAC, 1995). This workshop discussed many uses for ranking systems which are presented here.

One important current application is for regulators to use CRS to develop lists of chemicals which pose a potential threat to regional water quality and therefore need to be monitored and reported. Regulators also use CRS to determine which chemicals should be selected for bans or phase-outs. Setting priorities for chemical testing, pollution prevention strategies, product stewardship activities, industrial research and development, and waste minimization strategies are applications of CRS used by decision makers in both industry and regulatory agencies.

It was also noted at the SETAC workshop in 1995 that a CRS is a potentially useful

tool for determining the impact assessment on human health and the environment from the release inventory from a product Life Cycle Assessment (SETAC, 1995). The main advantage to using CRS for LCA impact assessment is that comparisons between chemicals released can be made based on their chemical, physical, and toxicological properties directly. Previous strategies involved aggregation with reference to one arbitrary toxic chemical. One toxicant was expressed in equivalency terms with reference to one selected chemical regardless of differences in mechanism of action or chemical properties. For example, using this aggregation scheme meant that chemicals such as trichloroethylene were being expressed as the equivalent of a calculated number of pounds of another chemical which may or may not be similar to it (for example in pounds of lead released). While this aggregation technique is understandable for impact categories such as acid rain (expressed as SO_2 equivalents) or global warming (expressed as CO_2 equivalents), aggregation does not work well for toxicants (Olsen, 1996). CRS allows risk assessors to quantify and compare a long list of chemicals to each other without the need for selecting a reference equivalent.

Chemical Ranking and Scoring Model

The CCPCT at the University of Tennessee Knoxville UTK developed a CRS in 1994 which is reported in the publication, "Chemical Hazard Evaluation For Management Strategies: A Method For Ranking And Scoring Chemicals By Potential Human Health and Environmental Impacts" (Davis et al., 1994). The CRS used in this thesis comes directly from this report with the exception of one scoring change for the no observable

adverse effect level (NOAEL). The SETAC Chemical Ranking and Scoring workshop identified the no observable effect concentration to be a useful and important toxicological endpoint (SETAC,1995). At the recommendation of researchers at the CCPCT one endpoint based on the consideration of frequency of publication in literature as reported in the ROADMAPS database is omitted. An additional endpoint involving the NOAEL is being added to the algorithm applied in this thesis (Swanson, Personal communication 1996). Whether the new scoring system for this endpoint will be adopted as it appears in this thesis for future use by the CCPCT will be at their discretion.

Scoring criteria consist of the three categories of human health, environmental effects, and exposure parameters. The toxicological endpoints considered for the human health and the environmental effects were the following:

Oral LD_{50} - The Oral Lethal Dose 50% is the concentration of a chemical in mg per mass of the animal in kg per day which results in the death of half of a group of rodents within 14 days.

Inhalation LC_{50} - The Inhalation Lethal Concentration 50% is the concentration of a chemical in parts per million (ppm) in air that will kill half of a group of animals when inhaled continuously for 8 hours or less.

Carcinogenicity is based on whether a chemical has ever possibly, probably, or definitely been shown to cause cancer in humans. These designations are determined by the International Agency for Research on Cancer (IARC) and the U.S. Environmental Protection Agency (U.S. EPA).

NOAEL - The No Observable Adverse Effect Level is the highest oral concentration in mg per mass of animal in kg (oral) or the highest concentration in air in mg/m^3 (inhalation) of a chemical which produced no toxic effects.

Fish LC_{50} - The Fish Lethal Concentration 50% is the concentration of a chemical in mg/L in water that kills half of the fish tested.

Fish NOEL - The Fish No Observable Effect Level is the highest concentration of a chemical in mg/L in water that does not produce toxic effects.

The exposure parameters considered in the CRS algorithm include the following properties of persistence and bioaccumulation:

BOD half-life - The Biological Oxygen Demand half-life is the time in days for a chemical to biodegrade such that the BOD in water is decreased to half the original amount.

HYD half-life - The Hydrolysis Half-life is the time in days for a chemical to decrease to half the original amount through a hydrolysis reaction in water at pH 7.

BCF - The Aquatic Bioconcentration Factor is the ratio of the concentration of a chemical in fish to its concentration in water (reported in logarithmic units).

The primary sources for data for the toxicological endpoints are the peer reviewed public access databases available on computer programs or through U.S. EPA publication. These database sources and the toxicological endpoints which are found in the databases are listed in Table 3. The specific sources for all the toxicological endpoints except for the oral NOAEL and inhalation NOAEL values for each chemical but tetrahydrofuran is referenced in the CCPCT report "Chemical Hazard Evaluation For Management

Table 3. Database Sources

DATABASE ACRONYM	TOXICOLOGICAL ENDPOINTS	REFERENCE
AQUIRE	fish LC_{50}, Daphnia EC_{50}	Aquatic Toxicity Information Retrieval Database (1994) U.S. EPA Environmental Research Laboratory. Technical Database Services, Inc. (TDS Numerica).
CESARS	acute oral LD_{50}, inhalation LD_{50}, fish LC_{50}, chronic pain (non-cancer) for UT model	Chemical Evaluation Search and retrieval System. Michigan Department of Natural Resources (MDNR). Maintained by MDNR and MOEE
ECDIN	acute oral LD_{50}, inhalation LD_{50}, BCF for inorganics	Environmental Chemicals Data and Information Network (ECDIN 1994) Environmental Research Programme of the Commission of the European Communities. Technical Database Services, Inc. (TDS Numerica).
HEAST	RfD, RfC	Health Effects Assessment Summary Tables (1994), U.S. EPA Office of Solid Waste and Emergency Response. EPA 540/R-94/020
HSDB	acute oral LD_{50}, inhalation LC_{50}, experimental log K_{ow}, 0, fish LC_{50}, IARC rating for carcinogens, chronic data (non-cancer) for UT model for non-TRI chemicals, special toxicity, BCF for inorganics	Hazardous Substances Data Bank (1993, 1994). The National Library of Medicine's Toxicology Data Network (TOXNET) System.
IRIS	EPA carcinogen classification, reference dose (RfD), reference concentration (RfC), chronic data (non-cancer) for UT model	Integrated Risk Information System (1994) U.S. EPA. The National Library of Medicine's Toxicology Data Network (TOXNET) System.
IRPTC database	chronic data (non-cancer) for UT model, BCF for inorganics	International Registry of Potentially Toxic Chemicals (IRPTC) PC Database Version 2.0 (1993) United Nations Environment Program.
IUCLID	Oral NOAEL, inhalation NOAEL	International Uniform Chemical Information Database (1994) European Chemicals Bureau
QSARS	BCF, hydrolysis half-life, BOD half-life	MicroQSAR version 2.0
RTECS	acute oral LD_{50}, inhalation LC_{50}	Registry of Toxic Effects of Chemical Substances (1992, 1993, 1994) National Institute of Occupational Safety and Health. The National Library of Medicine's Toxicology Data Network (TOXNET) System.
SAX Index	acute oral LD_{50}, inhalation LC_{50}, BCF for inorganics	Lewis, R. J. Sr., Ed. (1992). *Sax's Dangerous Properties of Industrial Materials*, 8th ed., Van Nostrand Reinhold, New York.

Strategies: A Method For Ranking And Scoring Chemicals By Potential Human Health and Environmental Impacts" (Davis et al., 1994). Tetrahydrofuran is a chemical which was not evaluated by the CCPCT report and all the toxicological endpoints for it were searched for in the standard databases. Specific sources and the values for the toxicological endpoints for the chemical tetrahydrofuran are listed in Table 4. The HEAST and IUCLID databases were used to collect the oral NOAEL and inhalation NOAEL endpoints. The specific sources for the NOAEL toxicological endpoints for each chemical are listed along with the values in Table 5.

When toxicological data is not available for a chemical, structure activity relationships are used to assign experimental endpoints from chemicals with similar functional groups. For certain aquatic endpoints such as fish LC50, the Quantitative Structure Activity Relationships (QSAR) are taken from the MicroQSAR version 2 computer program. The SETAC CRS workshop in 1995 identified QSARs to be useful and important for CRS endpoints because they can be easily obtained in the absence of experimental data (SETAC, 1995). If it was not possible to use structure activity relationships the conservative use of a maximum hazard value of 5 is used for the hazard value for that endpoint.

NOAEL Value

Direct toxicological endpoints are used for LCA analysis, and there are advantages and disadvantages to each value selected. Since no one endpoint is representative of all the potential adverse effects of a compound it is necessary to consider multiple

Table 4. Tetrahydrofuran Endpoints and Sources			
TETRAHYDROFURAN			
ENDPOINT	**TOXICOLOGICAL VALUE**	**SOURCE OF DATA**	**HAZARD VALUE**
HVoralLD50	rat 1650 mg/kg-day	RTECS	0.7
HVinhLC50	rat 21000ppm	RTECS	0.0
HVcarcin	none	none	5.0
HVnoael	oral rat 2.85 mg/kg-day	IUCLID	2.6
HVfish LC50	FHM96hr 2160 mg/L	HSDB	0.0
HVfishNoel	log(no Effect)=2.17	QSAR Microsystem	0.0
HVBod	520 days	QSAR Microsystem	2.5
HVhyd	1000 days	QSAR Microsystem	2.5
HVBcf	logBCF=-.13	QSAR Microsystem	1.0
RTECS - Registry of Toxic Effects of Chemical Substances			
IUCLID - International Uniform Chemical Information Database			
HSDB - Hazardous Substances Data Bank			
QSAR Microsystem - MicroQSAR version 2.0			

Table 5. Oral and Inhalation NOAEL Values					
CHEMICAL	**CAS NUMBER**	**NOAEL USED**	**UNITS**	**ROUTE of Administration**	**SOURCE**
1,3-Butadiene	106-99-0	18000.0	mg/m^3	inhalation	IUCLID
Acetone	67-64-1	100.0	mg/kg-day	oral	HEAST
Ammonia	7664-41-7	40.0	mg/m^3	inhalation	IUCLID
Ammonium Sulfate	7783-20-2	30.0	mg/m^3	inhalation	IUCLID
Asbestos (friable)	1332-21-4	none	none	none	none
Benzene	71-43-2	1.0	mg/kg-day	oral	IUCLID
Biphenyl	92-52-4	50.0	mg/kg-day	oral	HEAST
Carbon Disulfide	75-15-0	63.3	mg/m^3	inhalation	IUCLID
Chromium Compounds	20-06-4	2.4	mg/kg-day	oral	HEAST
Copper Compounds	20-08-6	0.0	mg/kg-day	oral	HEAST
Cumene	98-82-8	154.0	mg/kg-day	oral	HEAST
Cyclochexane	110-82-7	1517.0	mg/m^3	inhalation	IUCLID
Epichlorohydrin	106-89-8	9.6	mg/m^3	inhalation	IUCLID
Ethylbenzene	100-41-4	136.0	mg/kg-day	oral	IUCLID
Ethylene	74-85-1	none	none	none	none
Ethylene Glycol	107-21-1	200.0	mg/kg-day	oral	HEAST
Lead Compounds	20-11-1	none	none	none	none
m-Xylene	108-38-3	250.0	mg/kg-day	oral	HEAST
Manganese Compounds	20-12-2	0.1	mg/kg-day	oral	HEAST
Methanol	67-56-1	500.0	mg/kg-day	oral	HEAST
Methyl Ethyl Ketone	78-93-3	1771.0	mg/kg-day	oral	HEAST
Methyl Isobutyl Ketone	108-10-1	250.0	mg/kg-day	oral	HEAST
Naphthalene	91-20-3	none	none	none	none
Nickel Compounds	20-14-4	9.5	mg/kg-day	oral	HEAST
o-Xylene	95-47-6	250.0	mg/kg-day	oral	HEAST
p-Xylene	106-42-3	250.0	mg/kg-day	oral	HEAST
Phenol	108-95-2	60.0	mg/kg-day	oral	HEAST
Phosphoric Acid	7664-38-2	none	none	none	none
Propylene	115-07-1	8730.0	mg/m^3	inhalation	IUCLID
Propylene Oxide	75-56-9	363.0	mg/m^3	inhalation	IUCLID
Styrene	100-42-5	100.0	mg/kg-day	oral	IUCLID
Tetrachloroethylene	127-18-4	16.0	mg/kg-day	oral	IUCLID
Tetrahydrofuran	109-99-9	2.9	mg/kg-day	oral	IUCLID
Toluene	108-88-3	223.0	mg/kg-day	oral	HEAST
Trichloroethylene	79-01-6	500.0	mg/kg-day	oral	IUCLID
Vinyl Acetate	108-5-4	0.1	mg/kg-day	oral	IUCLID
Xylene (mix)	1330-20-7	250.0	mg/kg-day	oral	HEAST
Zinc Compounds	20-19-9	0.1	mg/kg/day	oral	HEAST
IUCLID -International Uniform Chemical Information Database of the European Chemicals Bureau					
HEAST - Health Effects Summary Tables of the U.S. EPA					

endpoints. For example, the oral LD_{50} and inhalation LC50 are important to consider for three reasons. These endpoints represent two different routes of administration, relate to the same gross endpoint (death of 50% of the test subjects), and are toxicological values which have been studied for many different chemicals and are usually available through standard databases. NOAEL values do not have all these advantages and could never replace the LD_{50} and LC_{50}, but they do serve as a complement to the lethal dose endpoints.

Two disadvantages of NOAEL values are that they are not studied as frequently or as precisely as the previous endpoints discussed. For the 38 chemicals in this study the oral NOAEL was found for 25 of them. The inhalation NOAEL was found for an additional 8 chemicals, and neither value was found for 5 chemicals. The brief descriptions of the experiment in the database indicated only 4 or 5 different concentrations were tested, and it is not apparent that an attempt was made to pinpoint a more exact concentration for no observed effect. For example a chemical might be tested for oral dose of 10, 100, 500, and 1000 mg/kg-day with a final oral NOAEL value of 10 mg/kg-day reported since no damage was observed. This lack of precision is probably due to the considerable expense of conducting animal studies.

Another reason NOAEL values are not considered a good basis for comparison by some researchers is that they are values which have completely different endpoints for the mechanism of action for each chemical. In addition, the gross endpoint is any adverse effect and does not specify the degree of harm (for example unpleasant taste versus

cellular neurological damage).

These criticisms of NOAELs are valid, but it is important to point out that they are still useful values for risk assessment when used in addition to other toxicological endpoints. It is also true that while the gross endpoint for LD_{50} and LC_{50} studies is death, the specific mechanism of action for the damage causing death is different for each chemical. The animals are dying from different causes (ie. lung damage for one chemical and stomach damage for another chemical), but the specific adverse effect is not taken into consideration even though the endpoints are being used for comparison.

The NOAEL value has been acknowledged by the newsletter of the Society of Environmental Toxicology and Chemistry to be a "useful and important toxicological endpoint" (SETAC, 1995). Several other CRS strategies include the oral NOAEL value as an endpoint. The Chemical Use Clusters Scoring System evaluates the NOAEL and the LOAEL (Least Observable Adverse effect level) (U.S. EPA, 1992). W. Klein et al. reported in their Environmental Hazard Ranking system consideration of oral NOEL (No Observable Effect Level), dermal NOEL, or inhalative NOEL (Klein et al., 1988). The NOAEL and the NOEL values are similar and could be used interchangeably. The U.S. EPA's Hazard Ranking System also considers NOAELs in its scoring system used to assess the threat associated with actual or potential releases of hazardous substances (Federal Register, 1988). The Ontario Ministry of Environment and Energy has a protocol for selecting substances for bans, phase-outs, or reductions. This system looks at persistence, bioaccumulation, and toxicity. This protocol does consider the oral NOEL

and the inhalation NOEL for toxicity scoring (OMEE, 1994).

Stig Olsen points out in his dissertation from the Technical University of Denmark that the effect observed by the NOAEL may not be the most severe effect as seen with higher doses, but it is a measure of safety based upon a critical effect for a chemical. This critical effect is defined as the toxic effect occurring at the lowest dose (Olsen, 1996). NOAEL is more a measure of potential toxicity than it is of actual toxicity. Most importantly the oral NOAELs are used to derive oral reference doses (RfDs) and inhalation NOAELs are used to derive inhalation reference concentrations (RfCs). The RfD and the RfC of a chemical are used to determine a "safe" exposure level (Olsen, 1996). The reference doses are calculated for non-carcinogens and non-mutagens and assume that there is a threshold below which exposure does not cause adverse health effects (U.S. EPA, 1994). Because NOAELs are used to derive the reference doses used for safety standards, they are a measure of safety as well as an indication of toxicity. NOAELs have a different contribution to make to risk assessment than lethal dose toxicity values, and it is appropriate to include their consideration.

Chemical Ranking and Scoring Algorithm

This section presents a description of the algorithm used in the CRS as derived by The CCPCT (Davis et al., 1994). The potential hazard of a released chemical to humans, terrestrial animals, and fish is evaluated and a numerical score is assigned. The scoring system for each toxicological endpoint is specific for that endpoint. In this CCPCT model, a hazard value (HV) is calculated for a chemical based on toxicity, persistence in

the environment, and tendency for bioaccumulation. A weighted hazard value based on exposure quantity is then calculated that combines this previous hazard value with an exposure parameter determined from the total quantity in pounds of chemicals released.

Several assumptions were made in the development of the algorithm. Since there is uncertainty in the accuracy of toxicity studies, it was assumed that these data are generally only accurate to within one order of magnitude. This justified the use of qualitative structure activity relationship (QSAR) derived data when experimental data were not available. Secondly, considering the range of toxicity and physical properties of the pollutants, the algorithm was constructed to give an approximate logarithmic response when necessary. This allowed pollutants of widely differing properties to be on the same scale and prevented one particular pollutant dominating over the others (Davis et al., 1994).

Additive terms (i.e., oral LD_{50}, inhalation LC_{50}, carcinogenicity, fish LC_{50}, fish NOEL, and chronic NOAEL) were given equal weighing by assigning a hazard value to each that ranged from 0 to 5. Cutoff values for end of the hazard value scale were chosen for the terms so that the hazard value for very high or very low toxicities would not exceed 5 or would not be less than 0 respectively. The choice of cutoff levels for assigning maximum or minimum hazard values adds a weighted judgement to the algorithm. Multiplicative terms for the exposure parameters BOD half-life, HYD half-life, and aquatic BCF were given hazard values that ranged from 1.0 to 2.5.

CHAPTER III

HAZARD VALUE DETERMINATION FOR TOXICOLOGICAL ENDPOINTS

Each toxicological endpoint is an additive effect and receives a hazard value (HV) between 0 (low toxicity) and 5 (high toxicity). The scoring for each endpoint is based on results of laboratory tests, carcinogenicity classifications, or QSARs. Between the minimum and maximum values of 0 and 5 the algorithm uses a continuous linear equation rather than a stepwise assignment of values. The separate hazard value equations for each toxicological endpoint are as follows:

Oral LD_{50} - Units in mg/kg-day

If $\log LD_{50} > 3.7$, then $HV_{orl\ LD50} = 0$;

If $\log LD_{50} \leq 0.7$, then $HV_{orl\ LD50} = 5$;

and $HV_{orl\ LD50} = (6.2 - 1.7 * \log LD_{50})$ for linear function.

Inhalation LC_{50} - Units in ppm.

Preferred test duration is 8 hours or less, scaled to 4 hours by this equation: $Concentration_1 * time_1 = concentration_2 * time_2$. For determining the HV_{LC50} the following equation is used:

If $\log LC_{50} > 4.0$, then $HV_{inhLC50} = 0$;

If $\log LC_{50} < 1.5$, then $HV_{inhLC50} = 5$;

and $HV_{inhLC50} = (8.0\text{-}2.0 * \log LC_{50})$ for linear function.

Carcinogenicity - For IARC Classifications:

If group 4, then $HV_{IARC} = 0$; If group 3, then $HV_{IARC} = 0$;

If group 2B, then $HV_{IARC} = 3.5$; If group 2A, then $HV_{IARC} = 4$;

If group 1, then $HV_{IARC} = 5$.

- For EPA Classifications:

If group E, then $HV_{EPA} = 0$; If group D, then $HV_{EPA} = 0$

If group C, then $HV_{EPA} = 1.5$; If group B2, then $HV_{EPA} = 3.5$;

If group B1, then $HV_{EPA} = 4$; If group A, then $HV_{EPA} = 5$.

If it has a HV_{EPA} rating and a HV_{IARC} rating does not equal 3,

then $HV_{Carcin} = (HV_{EPA} + HV_{IARC}) / 2$.

If it has a HV_{EPA} rating and a HV_{IARC} rating equal to 3, then $HV_{Carcin} = HV_{EPA}$

If it does not have a HV_{EPA} but it has a HV_{IARC} only, then $HV_{Carcin} = HV_{IARC}$

NOAEL - The protocol for HV_{NOAEL} involves two endpoints. The oral NOAEL value for a rodent is used first. If more than one value is presented in the database the most conservative (smallest) value was used. The inhalation NOAEL for a rodent is used if the oral value is not available.

- For oral rodent: Units in mg/kg-day

If $\log NOAEL_{orl} > 2.0$, then $HV_{NOAEL} = 0$

If $\log NOAEL_{orl} < -1.0$, then $HV_{NOAEL} = 5$

and $HV_{NOAEL} = -1.67 * \log(NOAEL_{orl}) + 3.33$ for linear function.

If oral rodent NOAEL is not available, then the inhalation NOAEL is used.

- For inhalation rodent: Units in mg/m^3

If $\log NOAEL_{inh} > 3.0$, then $HV_{NOAEL} = 0$

If $\log NOAEL_{inh} < 0.0$, then $HV_{NOAEL} = 5$

and $HV_{NOAEL} = - 1.67 * \log(NOAEL_{inh}) + 5.00$ for linear function.

Fish LC_{50} - Units in mg/L

If available the experimental values based on mortality to fathead minnows in a flow-through 96 hour test data are used first. If data from this test are unavailable then data from a flow-through 96 hour for another freshwater fish is selected The last tests considered are the static 96 hour fathead minnow test then the static 96 hour test for another freshwater fish. If no data are available use QSAR program selection. For any selection the following protocol is used:

If $\log LC_{50} \geq 3.0$, then $HV_{fishLC50} = 0$

If $\log LC_{50} < 0.0$, then $HV_{fishLC50} = 5$

and $Hv_{fishLC50} = -1.67*\log (fishLC_{50}) + 5.0$ for linear function.

Fish NOEL - Units in mg/L

Experimental data for the fish NOEL are used first. If the experimental values are not available then calculations with experimental or QSAR values are used. QSAR values of fish LC_{50} for inorganic compounds and organic compounds whose log of the octanol/water coefficient (K_{ow}) is greater than or equal to five are used to determine a fish NOEL. Use calculations with the fish LC_{50} for organic compounds whose log of the

octanol/water coefficient (K_{ow}) is less than two. The fish NOEL for the remaining organic chemicals is calculated using a continuous line equation.

If inorganic, then calculated fish NOEL = 1/20 Fish LC_{50}

If organic and log $K_{ow} \geq 5.0$, then calculated fish NOEL = 1/20 Fish LC_{50}

If organic and log $K_{ow} < 2.0$, then calculated fish NOEL = 1/4 Fish LC_{50}

Remaining organic compounds use this linear function:

Calculated fish NOEL = Fish LC_{50} / (5.3*log K_{ow} - 6.6)

Once a fish NOEL value is determined, the $HV_{fish\ NOEL}$ is as follows:

If log fish NOEL > 2.0, then $HV_{fish\ NOEL} = 0$

If log fish NOEL $\leq$ 1.0, then $HV_{fish\ NOEL} = 5$

and $HV_{fish\ NOEL}$ = 3.33 - 1.67 log fish NOEL for linear function.

Persistence and bioaccumulation are important for potential exposure and are included as multiplicative factors rather than additive factors. Each exposure factor is scored between a minimum value of 1.0 (low persistence and low bioaccumulation) and a maximum value of 2.5 (high persistence or high bioaccumulation). The separate hazard value equations for each exposure parameter endpoint are as follows:

BOD half-life - Units in days

The linear equation for BOD half-life uses the natural logarithm (ln) of the BOD half-life.

If the BOD half-life $\leq$ 4.0 days, then $HV_{BOD} = 1$

If the BOD half-life > 500 days, then $HV_{BOD} = 2.5$

and $HV_{BOD} = 0.311$ ln BOD half-life + 0.568

HYD half-life - Units in days

The linear equation for HYD half-life uses the natural logarithm (ln) of the HYD half-life.

If the HYD half-life ≤ 4.0 days, then $HV_{HYD} = 1$

If the HYD half-life > 500 days, then $HV_{HYD} = 2.5$

and $HV_{HYD} = 0.311$ ln HYD half-life + 0.568

BCF - Unitless ratio.

The linear equation for BCF uses the base ten logarithm of the BCF.

If log BCF ≤ 1.0, then $HV_{BCF} = 1$

If log BCF > 4.0, then $HV_{BCF} = 2.5$

and $HV_{BCF} = 0.5$ log BCF + 0.5 for the linear equation.

Determination of Total Hazard Value for Each Chemical

The total hazard value algorithm for a chemical without considering releases quantities is computed as follows:

Total Hazard Value =

(Human Health Effects + Environmental Effects) * (Exposure Factors)

where,

Human Health Effects = $HV_{orlLD50} + HV_{inhLC50} + HV_{Carcin} + HV_{NOAEL}$

Environmental Effects = $HV_{orlLD50} + HV_{fishLC50} + HV_{fishNOEL}$

Exposure Factors = $HV_{BOD} + HV_{HYD} + HV_{BCF}$

and,

HV = Hazard Value for the endpoints indicated in subscript

Human health effects in the algorithm range from 0.0 to 20.0 because of the maximum of 5.0 points for each of four endpoints. Environmental Effects range from 0.0 to 15.0 because of the maximum for 5.0 for each of three endpoints. Exposure Effects range from 3.0 to 7.5 because of a maximum of 2.5 for each of three endpoints. Overall the maximum possible total hazard value for a chemical independent of the amount released would be 262.5 (i.e, (20.0 + 15.0) * 7.5). To include consideration of the quantity of the compound released, the individual hazard values are multiplied by a weighted exposure multiplier which is based on the logarithm of the release amount in pounds.

Weighting by Exposure Quantity

The quantity of the chemical released is an important exposure parameter. The more of a pollutant released, the greater the possibility of exposure to the environment or to people, therefore the greater potential for harm. Human health and environmental damage may occur if a chemical of high toxicity is released in small amounts or if a chemical of low toxicity is released in large amounts. The range of quantities released can be many orders of magnitude. In the example analyzed in this thesis the exposures differ in range by seven orders of magnitude as indicated in Tables 1. and 2. (i.e. Olefin releases of 2.42×10^{-11} of cumene released to 1.98×10^{-04} of propylene released per pound of final product).

A large range in pounds of toxicants released is a problem for the algorithm since direct multiplication of the exposure quantities would unreasonably bias the total hazard value toward the chemicals with the highest amount released. Chemicals released in large quantities would have overwhelmingly large total hazard values and the importance of the toxicological endpoint values would not be reflected. Since the hazard value scores are bound between 0 and 5 for human and environmental health effects and between 1 and 2.5 for exposure factors it is necessary to bound the exposure quantities also. The range of 0 to 10 is selected for the exposure quantity which is used in the final equation as an exposure multiplier (EM). Taking the logarithm of the exposure in pounds results in negative values ranging from -9.18 to -3.56; therefore, it is necessary to add the number +13.0 to the logarithmic value in order to have a range between 0 and 10 as a multiplier.

The multiplicative factor used to weight toxicity hazard value totals for each compound according to the amount released is called the exposure multiplier (EM). The exposure multiplier is calculated for the HDPE data in the following equation:

Exposure Multiplier = log (release in pounds) + 13.0

The exposure multipliers for air, water, and land releases for the Olefin phase are presented in Table 6. The multipliers for air, water, and land release for the HDPE phase are presented in Table 7. If more than one media releases needs to be considered in the final total hazard value equation for a chemical, then the release amounts must be added together before the logarithm is taken.

It is important to note here that any products or production phases which are to be

Table 6. Olefin Air, Water, and Land Exposure Multipliers			
CHEMICAL	EMISSION SOURCE	LBS OF CHEMICAL PER LB OF PRODUCT	13+LOG10(LBS)
1,3-Butadiene	air	2.47E-05	8.39E+00
1,3-Butadiene	water/land	3.56E-09	4.55E+00
1,3-Butadiene	air/water/land	2.47E-05	8.39E+00
Acetone	air	5.26E-07	6.72E+00
Ammonia	air	6.05E-08	5.78E+00
Ammonia	water	1.02E-07	6.01E+00
Ammonia	air/water	1.63E-07	6.21E+00
Ammonium Sulfate	water	2.00E-05	8.30E+00
Asbestos (fri)	land	3.17E-05	8.50E+00
Benzene	air	5.37E-05	8.73E+00
Benzene	water/land	2.29E-06	7.36E+00
Benzene	air/water/land	5.60E-05	8.75E+00
Biphenyl	air	8.76E-08	5.94E+00
Biphenyl	water	3.32E-12	1.52E+00
Biphenyl	air/water	8.76E-08	5.94E+00
Carbon Disulfide	air	5.83E-07	6.77E+00
Carbon Disulfide	land	6.09E-09	4.78E+00
Carbon Disulfide	air/land	5.89E-07	6.77E+00
Chromium Compounds	water/land	1.69E-08	5.23E+00
Copper Compounds	water/land	2.83E-08	5.45E+00
Cumene	air	1.74E-07	6.24E+00
Cumene	water	2.42E-11	2.38E+00
Cumene	air/water	1.74E-07	6.24E+00
Cyclohexane	air	1.57E-06	7.20E+00
Epichlorohydrin	air	9.21E-08	5.96E+00
Ethylbenzene	air	6.08E-06	7.78E+00
Ethylbenzene	water/land	3.26E-07	6.51E+00
Ethylbenzene	air/water/land	6.41E-06	7.81E+00
Ethylene	air	2.77E-04	9.44E+00
Ethylene	water	7.07E-09	4.85E+00
Ethylene	air/water	2.77E-04	9.44E+00
Ethylene Glycol	air	1.42E-07	6.15E+00
Ethylene Glycol	water/land	6.99E-09	4.84E+00
Ethylene Glycol	air/water/land	1.49E-07	6.17E+00
Lead Compounds	land	6.14E-11	2.79E+00
m-Xylene	air	7.38E-07	6.87E+00
m-Xylene	water	3.07E-11	2.49E+00
m-Xylene	air/water	7.38E-07	6.87E+00

Table 6. (continued)			
CHEMICAL	EMISSION SOURCE	LBS OF CHEMICAL PER LB OF PRODUCT	13+LOG10(LBS)
Manganese Compounds	water	6.29E-09	4.80E+00
Methanol	air	2.26E-05	8.35E+00
Methanol	water	3.06E-09	4.49E+00
Methanol	air/water	2.26E-05	8.35E+00
Methyl Ethyl Ketone	air	1.52E-08	5.18E+00
Methyl Ethyl Ketone	land	3.00E-07	6.48E+00
Methyl Ethyl Ketone	air/land	3.15E-07	6.50E+00
Methyl Isobutyl Ketone	air	1.11E-07	6.05E+00
Methyl Isobutyl Ketone	land	2.62E-08	5.42E+00
Methyl Isobutyl Ketone	air/land	1.37E-07	6.14E+00
Naphthalene	air	2.23E-05	8.35E+00
Naphthalene	water/land	5.28E-07	6.72E+00
Naphthalene	air/water/land	2.28E-05	8.36E+00
Nickel Compounds	land	3.70E-07	6.57E+00
o-Xylene	air	3.45E-07	6.54E+00
p-Xylene	air	3.54E-07	6.55E+00
Phenol	air	2.78E-08	5.44E+00
Phenol	water	3.00E-04	9.48E+00
Phenol	air/water	3.00E-04	9.48E+00
Phosphoric Acid	air	3.48E-08	5.54E+00
Propylene	air	1.98E-04	9.30E+00
Propylene	water	5.25E-08	5.72E+00
Propylene	air/water	1.98E-04	9.30E+00
Styrene	air	2.12E-06	7.33E+00
Styrene	water/land	7.70E-08	5.89E+00
Styrene	air/water/land	2.20E-06	7.34E+00
Tetrachloroethylene	air	1.26E-10	3.10E+00
Toluene	air	1.63E-05	8.21E+00
Toluene	water/land	3.02E-04	9.48E+00
Toluene	air/water/land	3.18E-04	9.50E+00
Trichloroethylene	air	1.26E-10	3.10E+00
Vinyl Acetate	air	3.39E-08	5.53E+00
Xylene (mix)	air	2.45E-06	7.39E+00
Xylene (mix)	water/land	4.93E-06	7.69E+00
Xylene (mix)	air/water/land	7.38E-06	7.87E+00
Zinc Compounds	water/land	7.83E-08	5.89E+00

Table 7. HDPE Air, Water, and Land Exposure Multipliers			
CHEMICAL	**EMISSION SOURCE**	**LBS OF CHEMICAL PER LB OF PRODUCT**	**13+LOG10(LBS)**
Acetone	air	2.02E-09	4.31E+00
Ammonia	water	1.54E-08	5.19E+00
Asbestos (fri)	land	2.62E-07	6.42E+00
Carbon Disulfide	air	7.27E-08	5.86E+00
Chromium Compounds	air	1.02E-07	6.01E+00
Chromium Compounds	water/land	2.67E-06	7.43E+00
Chromium Compounds	air/water/land	2.78E-06	7.44E+00
Copper Compounds	water	7.88E-07	6.90E+00
Ethylene	air	2.24E-04	9.35E+00
Lead Compounds	water	1.08E-07	6.03E+00
Manganese Compounds	water	2.70E-06	7.43E+00
Methanol	air	1.85E-06	7.27E+00
Nickel Compounds	water	1.08E-07	6.03E+00
Phosphoric Acid	air	6.59E-10	3.82E+00
Propylene	air	7.35E-07	6.87E+00
Propylene Oxide	air	1.33E-06	7.12E+00
Tetrahydorfuran	air	1.33E-06	7.12E+00
Toluene	air	1.08E-06	7.03E+00
Xylene (mixed)	air	1.45E-08	5.16E+00
Zinc Compounds	water	3.76E-06	7.58E+00

compared to each other using this CRS method must use the same exposure multiplier calculation for each chemical released. Therefore, the calculation of the exposure multiplier must be computed separately for each data set taking into consideration the range of all the chemical exposure quantities. The purpose of the adjustment is to bound the exposure to a value between zero and ten and the specific calculation may vary depending on the exposure ranges for each given problem.

Final Equation Weighted by Releases

The final total hazard values for each chemical are calculated by multiplying the exposure multiplier by various hazard values depending on the media of release. The releases in pounds to the land are assumed to eventually end up in the water; therefore, the land releases are added to the water releases. It was also assumed that water and land releases would only result in oral exposures and in exposures to aquatic organisms. The HV_{LD50}, $HV_{fish\ LC50}$, HV_{NOAEL} (if based on the oral NOAEL), and $HV_{fishNOEL}$ are multiplied by the exposure multiplier calculated for the sum of the water and land releases. It is assumed that air releases would only result in inhalation exposure and would not result in oral exposures to the chemical. The HV_{LC50} and the HV_{NOAEL} (if based on the inhalation NOAEL) are multiplied by the exposure multiplier for the air releases. The HV_{Carcin} are multiplied by the exposure multiplier calculated for the sum of the air, water, and land releases. It is important to sum the releases in pounds from the various media before taking the logarithm and adding the integer adjustment number.

The final equation for the total hazard value for a chemical with an oral NOAEL value is as follows:

Total Hazard Value =

$$\left[(HV_{orlLD50} * EM_{water}) + (HV_{inhLc50} * EM_{air}) + (HV_{Carcin} * EM_{air+water}) + (HV_{NOAEL} * EM_{water}) \right.$$

$$\left. + \ (HV_{orlLD50} + HV_{fishLC50} + HV_{fishNOEL}) * EM_{water} \right]$$

$$* \ [HV_{BOD} + HV_{Hyd} + HV_{BCF}]$$

where,

HV = Hazard Value for the endpoints indicated in subscript

EM_{air} = Exposure Multiplier calculated from air releases

EM_{water} = Exposure Multiplier of water calculated from water + land releases

$EM_{air+water}$ = Exposure Multiplier of all media calculated from

air + water + land releases.

For a chemical with a HV_{NOAEL} based on an inhalation NOAEL, the HV_{NOAEL} is multiplied by the exposure multiplier calculated for air releases.

Determination of HV_{NOAEL}

The HV_{NOAEL} values are bound between 0 and 5. A minimum NOAEL value is selected as a cutoff value for the maximum hazard value (HV_{NOAEL} = 5). Any quantity below this minimum is also given a HV_{NOAEL} score of 5. A maximum NOAEL value is selected as a cutoff value for the minimum hazard value (HV_{NOAEL} = 0). Any quantity

above this maximum is also given a HV_{NOAEL} score of 0. The NOAEL values which fall between these minimum and maximum values are assigned a HV_{NOAEL} score based on a linear equation. To determine the minimum, maximum and the linear equation for the oral NOAEL hazard value a list of 179 rodent oral NOAEL values collected from information in the 1994 HEAST U.S. EPA database tables was studied. Expert opinion was use to determine the NOAEL values which represent the hazard value cutoffs ($HV_{NOAEL} = 0$ and $HV_{NOAEL} = 5$) (Bartmess, Personal communication 1996). The oral NOAEL values collected with the cutoff values in bold are presented in Table 8. The logarithm of the oral NOAEL values is a linear distribution.

From this line with X equal to the log(orlNOAEL) and Y equal to the $HV_{orlNOAEL}$ the following data points were selected:

For maximum hazard value: $Y = 5$ and $X = -1$

For minimum hazard value: $Y = 0$ and $X = +2$

and for values of X between -1 and +2 the line equation is:

$$\mathbf{Y = -1.67 * log(orlNOAEL) + 3.33}$$

To determine the minimum NOAEL, the maximum NOAEL and the linear equation for the inhalation NOAEL a list of 67 rodent inhalation NOAEL values were studied from the information in the 1994 HEAST U.S. EPA database tables and the 1994 IUCLID European Chemicals Bureau database. Again expert opinion was used to determine the NOAEL values which represent the inhalation hazard value cutoffs ($HV_{NOAEL} = 0$ and $HV_{NOAEL} = 5$) (Bartmess, Personal communication 1997). The inhalation NOAEL

Table 8. Oral NOAEL Values from HEAST					
ORAL NOAEL					
mg/kg-day					
5.00E-03	5.10E-01	3.00E+00	9.60E+00	3.00E+01	1.42E+02
8.40E-03	5.20E-01	3.00E+00	1.00E+01	3.00E+01	1.43E+02
2.00E-02	5.40E-01	3.10E+00	1.00E+01	3.00E+01	1.50E+02
2.50E-02	5.46E-01	3.10E+00	1.00E+01	3.20E+01	1.54E+02
2.50E-02	6.00E-01	3.50E+00	1.00E+01	3.20E+01	1.59E+02
2.60E-02	6.10E-01	3.90E+00	1.00E+01	3.58E+01	1.75E+02
3.00E-02	6.25E-01	4.00E+00	1.08E+01	4.30E+01	1.90E+02
3.30E-02	7.50E-01	4.20E+00	1.20E+01	4.40E+01	2.00E+02
5.00E-02	1.00E+00	5.00E+00	1.25E+01	5.00E+01	2.00E+02
5.00E-02	1.00E+00	5.00E+00	1.33E+01	5.00E+01	2.00E+02
5.50E-02	1.00E+00	5.00E+00	1.40E+01	5.00E+01	2.00E+02
6.00E-02	1.00E+00	5.00E+00	1.50E+01	5.00E+01	2.23E+02
7.00E-02	1.00E+00	5.00E+00	1.50E+01	5.00E+01	2.50E+02
8.00E-02	1.00E+00	5.00E+00	1.50E+01	5.00E+01	2.50E+02
9.00E-02	1.00E+00	5.00E+00	1.60E+01	5.57E+01	3.12E+02
9.00E-02	1.40E+00	5.00E+00	1.70E+01	5.60E+01	3.16E+02
1.00E-01	1.40E+00	5.00E+00	1.79E+01	6.00E+01	5.00E+02
1.50E-01	1.50E+00	5.01E+00	1.87E+01	7.50E+01	5.00E+02
2.00E-01	1.80E+00	5.85E+00	1.91E+01	8.27E+01	5.00E+02
2.00E-01	2.00E+00	6.00E+00	2.00E+01	8.30E+01	5.00E+02
2.30E-01	2.00E+00	7.10E+00	2.04E+01	9.14E+01	6.80E+02
2.30E-01	2.24E+00	7.30E+00	2.14E+01	9.60E+01	7.50E+02
2.60E-01	2.40E+00	7.30E+00	2.16E+01	**1.00E+02**	7.50E+02
3.00E-01	2.50E+00	7.50E+00	2.26E+01	1.00E+02	9.00E+02
3.30E-01	2.50E+00	7.50E+00	2.43E+01	1.00E+02	9.47E+02
3.40E-01	2.50E+00	8.00E+00	2.50E+01	1.15E+02	1.00E+03
4.00E-01	2.90E+00	8.00E+00	2.50E+01	1.25E+02	1.00E+03
4.30E-01	3.00E+00	8.45E+00	2.53E+01	1.25E+02	1.16E+03
5.00E-01	3.00E+00	9.20E+00	2.60E+01	1.25E+02	1.71E+03
5.00E-01	3.00E+00	9.50E+00	2.70E+01	1.25E+02	
Source: HEAST - Health Effects Assessment Summary Tables of the U.S. EPA					
BOLD denotes minimum and maximum hazard value cutoffs					

values with the cutoff values in bold are presented in Table 9. The logarithm of the inhalation NOAEL is a linear function. From this line with X equal to the log(inhNOAEL) and Y equal to the $HV_{inhNOAEL}$ the following data points were selected:

For maximum hazard value: $Y = 5$ and $X = 0$

For minimum hazard value: $Y = 0$ and $X = +3$

and for values of X between 0 and +3 the line equation is:

$$\mathbf{Y = - 1.67 * log(inhNOAEL) + 5.00}$$

Oral NOAEL versus Inhalation NOAEL

Oral and Inhalation NOAEL endpoints are not always available from standard databases and are not reported as very precise values. Therefore, the HV_{NOAEL} is only used once in the algorithm thus limiting its maximum contribution to the basic algorithm to only 5 out of 20 points for the human health effects portion (not considering exposure quantities). The preference for oral NOAEL values over inhalation values is based on the more frequent availability of the oral values in the HEAST database. Inhalation NOAEL values are used in the absence of oral NOAEL information because it is believed that using some experimentally determined values is more accurate than using no values at all. Converting inhalation values in mg/m^3 per day to oral values in mg/kg-day is not acceptable because this calculation ignores the importance of the route of administration to the mechanism of action of the chemical. The mechanism of action and the target organ of a chemical may be different depending upon whether the compound has a chance to pass from the intestines to the liver before going to target tissue. The liver can either

Table 9. Inhalation NOAEL from HEAST and IUCLID			
INHALATION NOAEL			
mg/m3			
9.00E-03	6.40E+00	7.30E+01	6.89E+02
1.00E-02	7.10E+00	7.50E+01	6.95E+02
6.60E-02	7.80E+00	9.30E+01	7.10E+02
2.00E-01	8.92E+00	9.52E+01	7.84E+02
2.00E-01	9.60E+00	1.02E+02	7.84E+02
9.80E-01	1.00E+01	1.05E+02	**1.00E+03**
1.00E+00	1.70E+01	1.21E+02	1.50E+03
1.40E+00	1.80E+01	1.21E+02	2.37E+03
1.50E+00	1.90E+01	1.60E+02	3.03E+03
1.70E+00	1.90E+01	1.71E+02	3.75E+03
2.20E+00	2.31E+01	1.76E+02	3.75E+03
2.50E+00	2.90E+01	2.87E+02	4.03E+03
2.50E+00	3.00E+01	3.63E+02	1.56E+04
3.75E+00	4.00E+01	3.80E+02	1.80E+04
4.31E+00	4.20E+01	4.33E+02	6.87E+04
4.50E+00	6.33E+01	5.00E+02	1.75E+05
6.00E+00	6.93E+01	5.25E+02	
HEAST - Health Effects Assessment Summary Tables of the U.S. EPA			
IUCLID - International Uniform Chemical Information Databases			
	of the European Chemicals Bureau		
BOLD denotes minimum and maximum hazard value cutoffs			

bioactivate compounds to make them more toxic or can detoxify compounds to make them less toxic. Separate minimum and maximum hazard score cutoff values and separate equations for scoring the NOAELs between the two cutoff values were developed for the HV_{NOAEL} for each of the two routes of administration.

Conversion of NOAEL Units Reported

Oral NOAEL values were presented in the databases in varying units. Usually the endpoints were reported in mg/kg-day which are recognized as standard toxicology units. Some of the endpoints were reported in mg/L concentration for oral ingestion of an aqueous solution by a rat in one day. These values were converted to mg/kg-day using information found in the book *Laboratory Animal Medicine* (Kohn, 1984). In one day an average rat consumes 95 ml of water per kg of body mass. Therefore, the following equation was used for dose unit conversion:

Dose in mg/kg-day = (Concentration mg/L of water)*(95ml/kg-day)*(.001L/ml)

Inhalation NOAEL values were also presented in the databases in varying units. Usually the endpoints were reported in mg of chemical per cubic meter of air (mg/m^3). Some of the endpoints were reported in parts per million (ppm) of air. To convert the ppm units to mg/m^3 it is necessary to use the ideal gas law, the gas constant in appropriate units, and the formula weight (FW in g/mole) of the chemical. From the ideal gas law it is calculated that the volume of one mole of the pure gas is 24.06 L at one atmosphere at room temperature. The ppm to mg/m^3 conversion equation is as follows:

$$\text{Dose in mg/m}^3 = \frac{(\text{Dose ppm}) * .001\text{L chemical}) * (1\ \text{mole}) * (\text{FWg/mole})}{(1\ \text{m}^3\text{air} * \text{ppm}) * (24.06\text{L chemical}) * (.001\text{g/mg})}$$

This dose conversion equation was applied to some studies which listed the inhalation NOAEL values in both ppm and mg/m^3 units and the conversion was consistent with these reported values.

NOAEL Values for Missing Data

If there was no value for the oral NOAEL or the inhalation NOAEL, the HV_{NOAEL} was assigned a value of 0 or 5 depending upon the value of the oral LD_{50}. For the 25 chemicals evaluated in this study with known oral NOAEL values, the oral LD_{50} and the oral NOAEL values were compared. For 18 values (72% of the total) the NOAEL value was less than the oral LD_{50} value, but within 2 orders of magnitude. Therefore, the oral LD_{50} was divided by 100 and used in the NOAEL equation to determine what a corresponding HV_{NOAEL} would be for that NOAEL value. If the calculated HV_{NOAEL} came out to be 0 then it was considered a true value and 0 was used. If the calculated HV_{NOAEL} came out to be 5 then it was considered a true value and 5 was used. If the calculated HV_{NOAEL} value was between 0 and 5 then a conservative value of 5 was used. For this example, the calculated HV_{NOAEL} for asbestos and ethylene was determined to be 0; therefore, values of 0 were assigned. The calculated HV_{NOAEL} for lead was 1.37, for naphthalene was 1.09, and for phosphoric acid was 1.35: therefore conservative values of 5 were assigned to each.

The specific NOAEL values collected or converted to a standard, the NOAEL units, the route of administration selected, and the final calculated HV_{NOAEL} for each chemical in both phases are listed in Table 10.

Table 10. Hazard Values for NOAEL				
CHEMICAL	NOAEL	UNITS	Route of Administration	HV NOAEL USED
1,3-Butadiene	18000.0	mg/m3	inhalation	0.0
Acetone	100.0	mg/kg-day	oral	0.0
Ammonia	40.0	mg/m3	inhalation	2.3
Ammonium Sulfate	30.0	mg/m3	inhalation	2.5
Asbestos (friable)	none	none	none	0.0
Benzene	1.0	mg/kg-day	oral	3.3
Biphenyl	50.0	mg/kg-day	oral	0.5
Carbon Disulfide	63.3	mg/m3	inhalation	2.0
Chromium Compounds	2.4	mg/kg-day	oral	2.7
Copper Compounds	none	mg/kg-day	oral	5.0
Cumene	154.0	mg/kg-day	oral	0.0
Cyclochexane	1517.0	mg/m3	inhalation	0.0
Epichlorohydrin	9.6	mg/m3	inhalation	3.4
Ethylbenzene	136.0	mg/kg-day	oral	0.0
Ethylene	none	none	none	0.0
Ethylene Glycol	200.0	mg/kg-day	oral	0.0
Lead Compounds	none	none	none	5.0
m-Xylene	250.0	mg/kg-day	oral	0.0
Manganese Compounds	0.14	mg/kg-day	oral	4.8
Methanol	500.0	mg/kg-day	oral	0.0
Methyl Ethyl Ketone	1771.0	mg/kg-day	oral	0.0
Methyl Isobutyl Ketone	250.0	mg/kg-day	oral	0.0
Naphthalene	none	none	none	5.0
Nickel Compounds	9.5	mg/kg-day	oral	1.7
o-Xylene	250.0	mg/kg-day	oral	0.0
p-Xylene	250.0	mg/kg-day	oral	0.0
Phenol	60.0	mg/kg-day	oral	0.4
Phosphoric Acid	none	none	none	5.0
Propylene	8728.0	mg/m3	inhalation	0.0
Propylene Oxide	363.0	mg/m3	inhalation	0.7
Styrene	100.0	mg/kg-day	oral	0.0
Tetrachloroethylene	16.0	mg/kg-day	oral	1.3
Tetrahydrofuran	2.9	mg/kg-day	oral	2.6
Toluene	223.0	mg/kg-day	oral	0.0
Trichloroethylene	500.0	mg/kg-day	oral	0.0
Vinyl Acetate	0.1	mg/kg-day	oral	5.0
Xylene (mix)	250.0	mg/kg-day	oral	0.0
Zinc Compounds	1.0	mg/kg-day	oral	5.0

CHAPTER IV

SUMMATION OF TOTAL HAZARD VALUES

Total Hazard values were calculated for each chemical released in both production phases. The hazard values for the individual human health effects, environmental health effects and exposure factors are calculated, summed, and presented in tables. The Olefin human health effects are presented in Table 11, the Olefin environmental effects are presented in Table 12, and the Olefin exposure factors are presented in Table 13. For the HDPE phase, the human health effects are listed in Table 14, the HDPE environmental health effects are listed in Table 15, and the HDPE exposure factors are listed in Table 16.

The final total hazard values for each chemical weighted by an exposure quantity are summed to calculate the overall total hazard values for each phase of manufacturing high density polyethylene plastic. The total hazard values for Olefin chemicals released are presented in Table 17. The summation of the total hazard values for the Olefin phase of high density polyethylene production is calculated to be 9159 and is also presented in Table 17. The total hazard values for the HDPE chemicals released are presented in Table 18. The summation of the total hazard values for the HDPE phase of high density polyethylene production is calculated to be 5418 and is also presented in Table 18. Comparing these overall hazard value scores it can be concluded that the manufacturing phase for the production of Olefin is more hazardous to the health of living organisms and to the environment than the final HDPE phase.

Table 11. Olefin Human Health Effects				
CHEMICAL	HVoralLD50	HVinhLC50	HVcarcin	HVnoael
1,3-Butadiene	0.3	0.0	3.5	0.0
Acetone	0.4	0.0	0.0	0.0
Ammonia	1.9	1.2	0.0	2.3
Ammonium Sulfate	0.4	5.0	0.0	2.5
Asbestos (friable)	0.0	0.0	5.0	0.0
Benzene	0.0	0.0	5.0	3.3
Biphenyl	0.3	5.0	0.0	0.5
Carbon Disulfide	0.4	1.6	0.0	2.0
Chromium Compounds	2.9	5.0	5.0	2.7
Copper Compounds	2.0	5.0	0.0	5.0
Cumene	0.4	0.2	0.0	0.0
Cyclohexane	0.0	2.6	0.0	0.0
Epichlorohydrin	3.5	2.6	3.8	3.4
Ethylbenzene	0.0	0.6	0.0	0.0
Ethylene	0.0	0.0	0.0	0.0
Ethylene Glycol	0.0	2.0	0.0	0.0
Lead Compounds	0.9	5.0	3.5	5.0
m-Xylene	0.0	0.7	0.0	0.0
Manganese Compounds	1.5	5.0	0.0	4.8
Methanol	0.0	0.0	0.0	0.0
Methyl Ethyl Ketone	0.4	0.3	0.0	0.0
Methyl Isobutyl Ketone	0.6	0.5	0.0	0.0
Naphthalene	0.6	5.0	1.0	5.0
Nickel Compounds	1.9	5.0	5.0	1.7
o-Xylene	0.0	0.7	0.0	0.0
p-Xylene	0.0	0.7	0.0	0.0
Phenol	1.6	4.7	0.0	0.4
Phosphoric Acid	0.9	5.0	0.0	5.0
Propylene	0.0	0.0	0.0	0.0
Styrene	1.2	1.2	3.5	0.0
Tetrachloroethylene	0.0	0.6	3.5	1.3
Toluene	0.0	0.4	0.0	0.0
Trichloroethylene	0.5	0.1	3.5	0.0
Vinyl Acetate	0.8	0.9	0.0	5.0
Xylene(mixed)	0.1	0.4	0.0	0.0
Zinc Compounds	0.0	5.0	0.0	5.0

Source: Gary Davis, Lori Kincaid, Mary Swanson, Terry Schultz, John Bartmess, Barbara Griffith, and Sheila Jones. "Chemical Hazard Evaluation For Management Strategies: A Method For Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts". University of Tennessee Center for Clean Products and Clean Technologies. June 1994.

Table 12. Olefin Environmental Health Effects			
CHEMICAL	**HVoralLD50**	**HVfish LC50**	**HVfishNoel**
1,3-Butadiene	0.3	4.0	3.3
Acetone	0.4	0.0	0.0
Ammonia	1.9	4.6	5.0
Ammonium Sulfate	0.4	0.0	0.0
Asbestos (friable)	0.0	0.0	0.0
Benzene	0.0	2.9	2.3
Biphenyl	0.3	4.6	4.9
Carbon Disulfide	0.4	0.3	0.0
Chromium Compounds	2.9	2.5	3.0
Copper Compounds	2.0	5.0	5.0
Cumene	0.4	3.7	3.8
Cyclohexane	0.0	3.9	4.0
Epichlorohydrin	3.5	2.4	1.8
Ethylbenzene	0.0	3.3	3.3
Ethylene	0.0	3.1	2.4
Ethylene Glycol	0.0	0.0	0.0
Lead Compounds	0.9	3.8	4.3
m-Xylene	0.0	3.0	3.0
Manganese Compounds	1.5	1.4	1.9
Methanol	0.0	0.0	0.0
Methyl Ethyl Ketone	0.4	0.0	0.0
Methyl Isobutyl Ketone	0.6	0.5	0.0
Naphthalene	0.6	3.7	3.7
Nickel Compounds	1.9	2.6	3.1
o-Xylene	0.0	3.0	2.8
p-Xylene	0.0	4.5	4.5
Phenol	1.6	2.4	1.8
Phosphoric Acid	0.9	1.9	2.4
Propylene	0.0	3.8	3.2
Styrene	1.2	4.0	3.9
Tetrachloroethylene	0.0	3.0	2.7
Toluene	0.0	2.4	2.3
Trichloroethylene	0.5	2.3	1.8
Vinyl Acetate	0.8	1.7	1.0
Xylene(mixed)	0.1	3.1	3.1
Zinc Compounds	1.2	2.7	3.2

Source: Gary Davis, Lori Kincaid, Mary Swanson, Terry Schultz, John Bartmess, Barbara Griffith, and Sheila Jones. "Chemical Hazard Evaluation For Management Strategies: A Method For Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts". University of Tennessee Center for Clean Products and Clean Technologies. June 1994.

Table 13. Olefin Exposure Factors			
CHEMICAL	**HVBod**	**HVhyd**	**HVBcf**
1,3-Butadiene	2.5	2.5	1.0
Acetone	1.2	2.5	1.0
Ammonia	1.3	2.5	1.0
Ammonium Sulfate	2.5	2.5	1.0
Asbestos (friable)	2.5	2.5	1.0
Benzene	1.3	2.5	1.1
Biphenyl	1.2	2.5	1.9
Carbon Disulfide	2.5	2.5	1.0
Chromium Compounds	2.5	2.5	1.7
Copper Compounds	2.5	2.5	1.0
Cumene	2.5	2.5	1.8
Cyclohexane	2.5	2.5	1.7
Epichlorohydrin	2.5	1.0	1.0
Ethylbenzene	1.3	2.5	1.5
Ethylene	1.3	2.5	1.0
Ethylene Glycol	1.3	2.5	1.0
Lead Compounds	2.5	2.5	1.4
m-Xylene	1.3	2.5	1.6
Manganese Compounds	2.5	2.5	1.0
Methanol	1.3	2.5	1.0
Methyl Ethyl Ketone	1.2	2.5	1.0
Methyl Isobutyl Ketone	1.2	2.5	1.0
Naphthalene	1.2	2.5	1.6
Nickel Compounds	2.5	2.5	1.3
o-Xylene	1.3	2.5	1.4
p-Xylene	1.3	2.5	1.5
Phenol	1.3	2.5	1.0
Phosphoric Acid	2.5	2.5	1.0
Propylene	1.3	2.5	1.0
Styrene	1.3	2.5	1.5
Tetrachloroethylene	2.5	2.5	1.3
Toluene	1.3	2.5	1.3
Trichloroethylene	2.5	2.5	1.2
Vinyl Acetate	1.3	2.5	1.0
Xylene(mixed)	1.3	2.5	1.5
Zinc Compounds	2.5	2.5	1.0

Source: Gary Davis, Lori Kincaid, Mary Swanson, Terry Schultz, John Bartmess, Barbara Griffith, and Sheila Jones. "Chemical Hazard Evaluation For Management Strategies: A Method For Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts". University of Tennessee Center for Clean Products and Clean Technologies. June 1994.

Table 14 HDPE Human Health Effects				
CHEMICAL	**HVoralLD50**	**HVinhLC50**	**HVcarcin**	**HVnoael**
Acetone	0.4	0.0	0.0	0.0
Ammonia	1.9	1.2	0.0	2.3
Asbestos (friable)	0.0	0.0	5.0	0.0
Carbon Disulfide	0.4	1.6	0.0	2.0
Chromium Compounds	2.9	5.0	5.0	2.7
Copper Compounds	2.0	5.0	0.0	5.0
Ethylene	0.0	0.0	0.0	0.0
Lead Compounds	0.9	5.0	3.5	5.0
Manganese Compounds	1.5	5.0	0.0	4.8
Methanol	0.0	0.0	0.0	0.0
Nickel Compounds	1.9	5.0	5.0	1.7
Phosphoric Acid	0.9	5.0	0.0	5.0
Propylene	0.0	0.0	0.0	0.0
Propylene Oxide	1.4	1.5	4.0	0.7
Tetrahydrofuran	0.7	0.0	5.0	2.6
Toluene	0.0	0.4	0.0	0.0
Xylene (mixed)	0.1	0.4	0.0	0.0
Zinc Compounds	0.0	5.0	0.0	5.0

Source: Gary Davis, Lori Kincaid, Mary Swanson, Terry Schultz, John Bartmess, Barbara Griffith, and Sheila Jones. "Chemical Hazard Evaluation For Management Strategies: A Method For Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts". University of Tennessee Center for Clean Products and Clean Technologies. June 1994.

Table 15. HDPE Environmental Health Effects			
CHEMICAL	**HVoralLD50**	**HVfish LC50**	**HVfishNoel**
Acetone	0.4	0.0	0.0
Ammonia	1.9	4.6	5.0
Asbestos (friable)	0.0	0.0	0.0
Carbon Disulfide	0.4	0.3	0.0
Chromium Compounds	2.9	2.5	3.0
Copper Compounds	2.0	5.0	5.0
Ethylene	0.0	3.1	2.4
Lead Compounds	0.9	3.8	4.3
Manganese Compounds	1.5	1.4	1.9
Methanol	0.0	0.0	0.0
Nickel Compounds	1.9	2.6	3.1
Phosphoric Acid	0.9	1.9	2.4
Propylene	0.0	3.8	3.2
Propylene Oxide	1.4	0.9	0.2
Tetrahydrofuran	0.7	0.0	0.0
Toluene	0.0	2.4	2.3
Xylene (mixed)	0.1	3.1	3.1
Zinc Compounds	1.2	2.7	3.2

Source: Gary Davis, Lori Kincaid, Mary Swanson, Terry Schultz, John Bartmess, Barbara Griffith, and Sheila Jones. "Chemical Hazard Evaluation For Management Strategies: A Method For Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts". University of Tennessee Center for Clean Products and Clean Technologies. June 1994.

Table 16. HDPE Exposure Factors			
CHEMICAL	**HVBod**	**HVhyd**	**HVBcf**
Acetone	1.2	2.5	1.0
Ammonia	1.3	2.5	1.0
Asbestos (friable)	2.5	2.5	1.0
Carbon Disulfide	2.5	2.5	1.0
Chromium Compounds	2.5	2.5	1.7
Copper Compounds	2.5	2.5	1.0
Ethylene	1.3	2.5	1.0
Lead Compounds	2.5	2.5	1.4
Manganese Compounds	2.5	2.5	1.0
Methanol	1.3	2.5	1.0
Nickel Compounds	2.5	2.5	1.3
Phosphoric Acid	2.5	2.5	1.0
Propylene	1.3	2.5	1.0
Propylene Oxide	1.3	1.0	1.0
Tetrahydrofuran	2.5	2.5	1.0
Toluene	1.3	2.5	1.3
Xylene (mixed)	1.3	2.5	1.5
Zinc Compounds	2.5	2.5	1.0

Source: Gary Davis, Lori Kincaid, Mary Swanson, Terry Schultz, John Bartmess, Barbara Griffith, and Sheila Jones. "Chemical Hazard Evaluation For Management Strategies: A Method For Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts". University of Tennessee Center for Clean Products and Clean Technologies. June 1994.

Table 17. Olefin Total Hazard Values				
CHEMICAL	**Human Health**	**Environmental Health**	**Exposure**	**TOTAL HV**
	Effects	**Effects**	**Factor**	
Naphthalene	87.7	53.8	5.3	748.7
Nickel Compounds	56.5	49.9	6.3	670.4
Chromium Compounds	55.4	43.9	6.7	660.4
Copper Compounds	38.2	65.4	6.0	621.5
Benzene	68.3	38.3	4.9	516.6
Styrene	41.6	53.6	5.2	496.5
Ammonia	31.7	69.1	4.8	478.6
Phenol	44.5	55.0	4.8	472.7
Zinc Compounds	29.5	37.1	7.0	466.3
1,3-Butadiene	30.7	34.6	6.0	392.6
Lead Compounds	26.2	25.1	6.4	327.8
Manganese Compounds	30.0	23.0	6.0	318.2
Xylene(mixed)	3.7	48.5	5.2	273.5
Epichlorohydrin	58.5	0.0	4.5	263.0
Biphenyl	30.9	14.9	5.6	258.1
Asbestos (friable)	42.5	0.0	6.0	255.0
Ethylbenzene	4.7	43.0	5.3	253.1
Toluene	3.3	44.6	5.1	244.0
Propylene	0.0	40.0	4.8	191.4
Carbon Disulfide	26.3	3.3	6.0	177.7
Phosphoric Acid	27.7	0.0	6.0	166.2
Cumene	2.2	18.8	6.8	142.4
Ethylene	0.0	26.7	4.8	127.5
Cyclohexane	18.7	0.0	6.7	124.8
m-Xylene	4.8	14.9	5.3	105.2
Tetrachloroethylene	12.7	0.0	6.3	80.0
Trichloroethylene	11.2	0.0	6.2	68.6
Ethylene Glycol	12.3	0.0	4.8	58.4
Methyl Isobutyl Ketone	6.3	6.0	4.7	56.9
Ammonium Sulfate	3.3	3.3	6.0	39.8
Methyl Ethyl Ketone	4.1	2.6	4.7	31.3
p-Xylene	4.6	0.0	5.3	24.3
Vinyl Acetate	5.0	0.0	4.8	23.6
o-Xylene	4.6	0.0	5.1	23.5
Acetone	0.0	0.0	4.7	0.0
Methanol	0.0	0.0	4.8	0.0
TOTAL				**9159**

Table 18. HDPE Total Hazard Values				
CHEMICAL	**Human Health Effects**	**Environmental**	**Exposure Factor**	**TOTAL HV**
Chromium Compounds	108.9	62.4	6.7	1138.7
Copper Compounds	48.3	82.8	6.0	786.2
Lead Compounds	56.7	54.3	6.4	709.4
Nickel Compounds	51.9	45.9	6.3	615.8
Zinc Compounds	37.9	47.7	7.0	599.2
Manganese Compounds	46.4	35.7	6.0	492.7
Ammonia	9.9	59.7	4.8	330.2
Tetrahydorfuran	35.6	0.0	6.0	213.7
Asbestos (fri)	32.1	0.0	6.0	192.5
Propylene Oxide	44.2	0.0	3.3	143.5
Phosphoric Acid	19.1	0.0	6.0	114.6
Carbon Disulfide	9.4	0.0	6.0	56.3
Toluene	2.8	0.0	5.1	14.3
Xylene (mixed)	2.1	0.0	5.2	10.8
Acetone	0.0	0.0	4.7	0.0
Ethylene	0.0	0.0	4.8	0.0
Methanol	0.0	0.0	4.8	0.0
Propylene	0.0	0.0	4.8	0.0
TOTAL				**5418**

These overall summations should not be treated as numerical values which can be divided into a whole or into each other and compared directly to each other mathematically. These sums are derived from relative ranking sores which were meant to be compared to each other for the purpose of ordering only. For example, the Olefin phase produces a much higher total hazard value than the HDPE phase but it would not be accurate to assume that this first phase is 1.7 times more hazardous.

The more conservative choice of using the maximum hazard value of 5 for health and environmental effects and 2.5 for exposure factors for toxicological endpoints with missing data offers the greatest environmental protection. Assigning one maximum value also avoids the need to report the total hazard values for each chemical in a range. Summing individual values which are reported in a range is awkward because as the totals are summed the ranges are also added together. For production processes with similar environmental impacts large ranges could potentially overlap and make comparisons difficult or meaningless.

The sensitivity of the algorithm was tested with all the unknown HV_{NOAEL} values defaulted to 0 and then defaulted to 5. For the $HV_{NOAEL} = 0$ default sensitivity test, the Olefin phase total hazard value was 8892 and the HDPE phase total hazard value was 5225. For the $HV_{NOAEL} = 5$ default sensitivity test, the Olefin phase total hazard value was 9530 and the HDPE phase total hazard value was 5611. The conclusion that the Olefin Phase is more environmentally hazardous than the HDPE is the same in all cases;

therefore, the algorithm is not sensitive to either a default of 0 or to a default of 5 used for the 5 unknown NOAEL endpoints out of the 38 total NOAEL endpoints in this example.

CHAPTERV

CONCLUSION

The relative potential hazards from chemical releases to air, water, and land for the manufacture of a plastic material was calculated using a chemical ranking and scoring system. The manufacturing process was divided into two phases (Olefin and HDPE) so that the individual phases could be compared and the most environmentally harmful production phase could be identified. The chemicals were ranked based on their properties of toxicity, persistence, and bioaccumulation and on their quantity released in pounds of chemical per pound of final product. The total hazard values calculated for each chemical release were summed and these two totals were directly compared. In this example, the Olefin phase had a total hazard value of 9159 which was higher than the 5418 value for the HDPE phase. Therefore, it was determined by the chemical ranking and scoring system applied to the Life Cycle Assessment release inventory for the production of high density polyethylene plastic that the Olefin phase is potentially more hazardous than the HDPE phase.

A modified chemical ranking and scoring system was developed as a tool to identify environmental and human health hazards of a manufacturing process. The chemical ranking and scoring system was based on the system developed by the Center for Clean Products and Clean Technologies. This new tool included the toxicological endpoint of the No Observable Adverse Effect Level (NOAEL). NOAELs are not strong enough

indicators of direct toxicity to be used exclusively to determine the overall impact of each chemical release. NOAEL values are an indication of potential toxicity; therefore, they are useful and appropriate toxicological endpoints to consider along with several other toxicological endpoints when assessing potential impact.

This Life Cycle Assessment information could be valuable to companies trying to reduce the overall adverse environmental impacts of their products. Impact assessments from Life Cycle Assessment of chemical releases could help identify the production phases which should be targeted for attention. Industry could also use the chemical ranking and scoring system applied to Life Cycle Assessment inventories to compare different base materials in order to identify which of these materials would be best to use in the manufacture of their products.

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Susan Sharp grew up in Southern California and graduated from Marina High School in Huntington Beach in 1975. She attended the University of California, Riverside from 1975 to 1978. She graduated with a B.S. Degree in Life Science from the University of Missouri, Rolla in 1980. She worked in the laboratory of the Phelps County Memorial Hospital from 1978 to 1981 and in the Life Science laboratory at the University of Missouri from 1981 to 1982. Susan moved to Oak Ridge, Tennessee in 1983, and she attended the University of Tennessee, Knoxville part-time for several years while working on her Master's Degree. Susan is married to Richard Ward and has two daughters.