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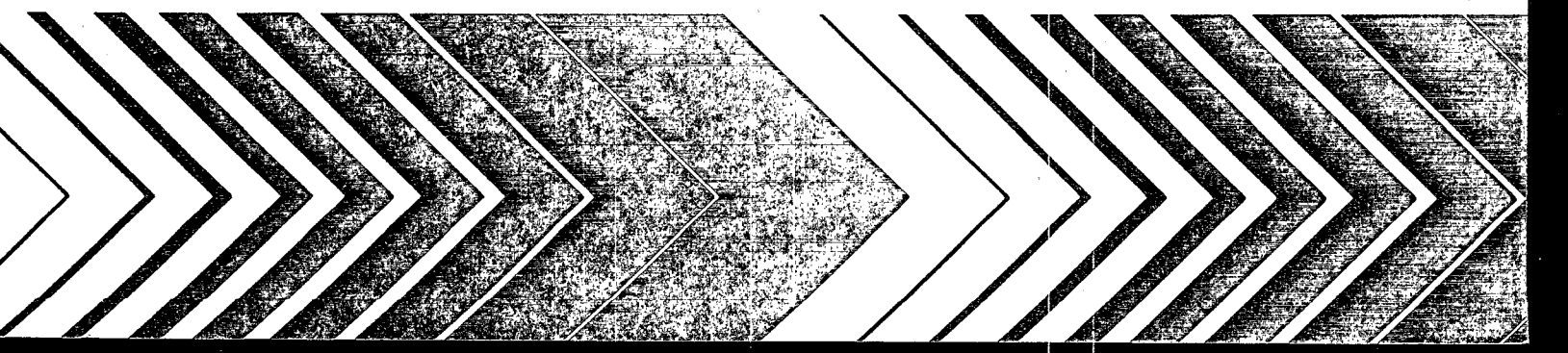
A Method for Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts



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CHEMICAL HAZARD EVALUATION FOR MANAGEMENT STRATEGIES:

A METHOD FOR RANKING AND SCORING CHEMICALS BY POTENTIAL HUMAN HEALTH AND ENVIRONMENTAL IMPACTS

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DISCLAIMER

The information in this document has been funded wholly by the United States Environmental Protection Agency under Cooperative Agreement CR #816735-01-0, to the University of Tennessee's Center for Clean Products and Clean Technologies. It has been subject to peer and administrative review, and has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

FOREWORD

Today's rapidly developing and changing technologies and industrial products and practices frequently carry with them the increased generation of materials that, if improperly dealt with, can threaten both public health and the environment. The U.S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. These laws direct EPA to perform research to define our environmental problems, measure the impacts, and search for solutions.

The Risk Reduction Engineering Laboratory is responsible for planning, implementing, and managing research, development and demonstration programs to provide an authoritative, defensible engineering basis in support of the policies, programs, and regulations of the EPA with respect to drinking water, wastewater, pesticides, toxic substances, solid and hazardous wastes, and Superfund-related activities. This publication is one of the products of that research and provides a vital communication link between the researcher and the user community.

This report, *Chemical Hazard Evaluation for Management Strategies: A Method for Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts*, funded through the Pollution Prevention Research Branch, is a major project in the area of the Cleaner Products Program in researching methods to support the design and development of products whose manufacture, use, recycle and disposal represent reduced impacts on the environment.

This report presents a method for chemical ranking and scoring, designed for priority setting, to identify specific chemicals as priorities for assessment of safer substitutes for major uses. This methodology was developed for use in the project *The Product Side of Hazardous Waste Reduction: Evaluating the Potential for Safe Substitutes*. A report on this project is published under separate cover. Risk-based chemical ranking and scoring combines an assessment of both the toxic effects of chemicals and the potential exposure to those chemicals, to provide a relative evaluation of risk. Risk assessment is an integral part of the environmental equation for successful protection and sustainability. The reader is encouraged to contact the authors or project officer for more information concerning this project and report.

E. Timothy Oppelt, Director
Risk Reduction Engineering Laboratory

ABSTRACT

Between 60,000 and 100,000 of the over than 8,000,000 chemicals listed by the Chemical Abstracts Services Registry are commercially produced and are potential environmental pollutants. Risk-based evaluation for these chemicals is often required to evaluate the potential impacts of chemical releases, for priority setting for regulatory action, for business decisions and to set priorities for pollution prevention. During the last decade, there have been vast improvements in the methods used to assess chemical toxicity and environmental fate and to interpret these data within a risk assessment framework. There is still a need, however, for generally accepted and widely used tools for setting priorities and providing consistency across environmental programs.

Risk ranking and scoring systems can be used to focus attention and resources on the most significant hazards posed by industrial facilities, products or hazardous material sites. Risk-based chemical ranking and scoring combines an assessment of both the toxic effects of chemicals (human and/or environmental) and the potential exposure to those chemicals to provide a relative evaluation of risk.

This method provides an approximate ranking of direct chemical hazards to human health and the environment based on their relative toxicity and the potential for exposure. The method does not include an evaluation of secondary global impacts such a ozone depletion and global warming.

An algorithm has been developed to combine and weight evaluation criteria to provide a working tool that ranks chemicals according to their potential human health and ecotoxic effects, and their potential environmental persistence and bioaccumulation. This report presents methodology for doing ranking at a first, or screening-level, tier.

This report was submitted in partial fulfillment of Cooperative Agreement CR #816735-01-0 by the University of Tennessee's Center for Clean Products and Clean Technologies, under the sponsorship of the U.S. Environmental Protection Agency. This work covers a period from September 10, 1990 to September 9, 1994, and was completed as of August, 1994.

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LIST OF ACRONYMS

ATSDR: Agency for Toxic Substances and Disease Registry
BCF: bioconcentration factor
BOD: biological oxygen demand
CLSES: Center for Lake Superior Environmental Studies
CMR: Critical Materials Register
DWCD: Drinking Water Criteria Documents (EPA)
EC_{50}: median effect concentration; the concentration at which 50 percent of the test population exhibit a specified response during a specified time period
EPA: United States Environmental Protection Agency
GENETOX: Genetic Toxicity Chemical Information System (on-line database)
HAD: Health Assessment Document (EPA)
HEA: Health Effects Assessment (EPA)
HEED: Health and Environmental Effects Document (EPA)
HEEP: Health and Environmental Effects Profile (EPA)
HSDB: Hazardous Substance Data Bank, National Library of Medicine (on-line database)
IARC: International Agency for Research on Cancer
IPCS: International Programme on Chemical Safety
K_{ow}: octanol-water partitioning coefficient
LC_{50}: median lethal concentration; the concentration at which 50 percent of the test population die during a specified time period
LD_{50}: median lethal dose; the dose at which 50 percent of the test population die during a specified time period
NOEL: no observable effect level
POTW: publicly owned treatment works
QSAR: quantitative structure-activity relationship
RTECS: Registry of Toxic Effects of Chemical Substances (on-line database)
RWF: release weighting factor
SAR: structure-activity relationship
SARA: Superfund Amendments and Reauthorization Act
SMILES: Simplified Molecular Input Line Entry System
TRI: Toxic Release Inventory
wHV: release-weighted hazard value
WMS: Wet Milieugevaarlijke Stoffen
WOE: weight of evidence

CHAPTER 1

INTRODUCTION

Between 60,000 and 100,000 of the over 8,000,000 chemicals listed by the Chemical Abstracts Services Registry are commercially produced and are potential environmental pollutants. Some kind of risk-based evaluation for these chemicals is often required to evaluate the potential impacts of chemical releases, for priority setting for regulatory action, for business decisions and to set priorities for pollution prevention. During the last decade there have been vast improvements in the methods used to assess chemical toxicity and environmental fate and to interpret these data within a risk assessment framework. There is still a need, however, for generally accepted and widely used tools for setting priorities and providing consistency across environmental programs. To date, we have relied upon a multitude of approaches, some lacking any scientific basis. Chemical have been selected for some regulatory programs, for example, with little systematic evaluation.

Risk ranking and scoring systems can be used to focus attention and resources on the most significant hazards posed by industrial facilities, products or hazardous material sites. Risk-based chemical ranking and scoring combines an assessment of both the toxic effects of chemicals (human and/or environmental) and the potential exposure to those chemicals to provide a relative evaluation of risk. Along with toxicity and exposure, ranking and scoring systems may include some measure of economic impact and/or societal value.

Risk-based chemical ranking and scoring combines an assessment of both the toxic effects of chemicals and the potential exposure to those chemicals to provide a relative evaluation of risk.

The University of Tennessee Center for Clean Products and Clean Technologies developed the chemical ranking and scoring method in this report under Environmental Protection Agency (EPA) Cooperative Agreement CR 816735, *The Product Side of Hazardous Waste Reduction: Evaluating the Potential for Safe Substitutes*. The method was designed for priority setting, to identify specific chemicals as priorities for assessment of safer substitutes for major uses. The method

provides an approximate ranking of direct chemical hazards to human health and the environment based on their relative toxicity and the potential for exposure. The method does not include an evaluation of secondary global impacts such as ozone depletion and global warming.

MAJOR RESEARCH TASKS

In the development of the chemical ranking method, three major research tasks were performed:

- compiling available experimental data and selecting estimation methods for those instances when experimental data were absent;
- formulating scoring criteria, which, individually or in combination, could be used to estimate the toxic effects of chemicals and the potential for exposure; and
- developing an algorithm to combine and weight evaluation criteria to provide a working tool that ranks chemicals according to their potential human health and ecotoxic effects, and their potential environmental persistence and bioaccumulation.

The method was demonstrated using the chemicals for which toxic chemical release reporting is made in the Toxic Release Inventory (TRI) as required under Section 313 of Title III of the Superfund Amendments and Reauthorization Act (SARA) of 1986. Selected high-volume pesticides, as determined by annual pesticide usage data, were also included.

Chapter 2 of this report presents an overview of the sources of toxicity and exposure data used to develop the chemical ranking and scoring method. Chapter 3 discusses the types of scoring criteria selected for the model, including human health effects criteria, environmental effects criteria and exposure parameters. Chapter 4 is a detailed description of the algorithm. Chapter 5 presents the results of the algorithm when it is demonstrated on the TRI chemicals and high-volume pesticides. Several *a priori* conditions that were incorporated into the design of the model, and the tiered approach envisioned for the model are discussed below.

A PRIORI CONDITIONS

Several *a priori* conditions were incorporated into the development of this scheme. First, it was determined that whatever the framework of the chemical ranking method, the final tool was to be sufficiently flexible so it could be modified as experience was gained and the validation process progressed. Second, at no time was the process to become so mechanical as to be isolated from expert judgment. Finally, although it was not necessary to separate human health and environmental effects according to different endpoints, this would make the algorithm more transparent. Because it would be easier to categorize these endpoints on the front end, the aggregation of information would be done late in the processing.

The screening tier was designed to avoid false negatives, including rather than eliminating chemicals of possible concern. The confirmation tier should be designed to avoid false positives and identify only chemicals of concern.

TIERED APPROACH

The quantity and intricacy of the information required for a complete assessment of each chemical, as well as the time and resources needed to procure and process this information, can be prohibitive. Thus, a tiered approach

was adopted with the method presented here being the first, or screening-level, tier. The advantage of the tiered approach is that it reduces the number of chemicals being evaluated as the depth, breadth and quality of the required information increases. While any number of tiers may be employed, a two-tiered approach that consists of a screening tier and a confirmation tier should be sufficient.

The screening tier was formulated to rely on more readily available and/or easily estimated information, while the confirmation tier should be formulated to define the potential for specific human health, environmental and/or global effects. Also, the screening tier was designed to include rather than eliminate chemicals of possible concern (avoid false negatives); the confirmation tier should be designed to identify only chemicals of concern (avoid false positives). The information used at the screening tier was designed to be a partial assessment and sufficient to prioritize pollutants. Using the results of the screening tier, one should be able to identify priority chemicals and move them to the yet-to-be-designed confirmation tier, or identify chemicals of lower concern and remove them from further consideration. The information used at the confirmation tier should be designed to be sufficient to render a full assessment or flag the chemical as having insufficient data for proper analysis. In this way, information used in the screening tier will be carried forward to the confirmation tier.

CHAPTER 2

SOURCES OF TOXICITY AND EXPOSURE DATA

Although some data are available in the open literature for many of the chemicals listed in the TRI, complete quantification of even a limited number of toxicological endpoints is rare. One of the main obstacles to the development and use of any chemical ranking or scoring system is the problem of what to do about this missing data. The types of scoring criteria used and the design of the algorithm for combining the criteria depend in large part on whether experimental data are available or can be estimated with an acceptable degree of accuracy.

One of the main obstacles to the development and use of any chemical ranking or scoring system is the problem of missing data.

Some chemical ranking and scoring systems incorporate expert judgment to fill data gaps, either through analytical tools based on structure analysis, or through ad hoc expert judgment. Other systems avoid the use of non-experimental data to fill data gaps by defaulting to endpoints for which data exists or relying upon the most sensitive endpoint as the measure of chemical risk. (See Davis, et al., (1994b) for a comparison of data selection approaches for approximately 50 ranking and scoring systems.) The latter method presents obvious problems when little or no experimental data exist on a chemical. It also does not necessarily encourage further testing of compounds, since it is unlikely that a score for a chemical can be lowered by filling data gaps.

The chemical ranking method described in this report relies on peer-reviewed experimental data from sources such as the Hazardous Substances Data Bank (HSDB) whenever possible. In the absence of experimental data, structure analysis is used to estimate missing data to ensure that highly toxic chemicals do not receive a low ranking simply because they have not been tested. (For further information concerning the database, contact the University of Tennessee Center for Clean Products and Clean Technologies)

THE USE OF STRUCTURE ANALYSIS

Structure analysis can be qualitative or quantitative in nature. Qualitative structure analysis involves evaluation of the molecular structure of a chemical and the use of qualitative correlations of particular molecular substructures and/or functional groups with specific effects. In this model, qualitative structure analyses are classified as structure-activity relationships (SARs). SARs are often used to make judgments concerning the potential health effects of a pollutant. Quantitative structure analysis involves the development and computerization of quantitative structure-property, property-property, structure-activity and property-activity relationships, hereafter referred to collectively as quantitative structure-activity relationships or QSARs. QSARs are widely accepted methods to estimate missing data for many endpoints, particularly physicochemical properties and environmental effects.

Both QSARs and SARs are based on the working hypothesis of "Guilt by Association," which says chemicals with similar molecular structures have similar physicochemical properties and, therefore, similar biological activities. Despite potential short-comings, structure-activity is presently the best means of supplying missing data. This is certainly the case if the processing of information takes on a less quantitative nature where an order or half-order of magnitude is sufficiently accurate. Additionally, data for some toxicological endpoints, such as developmental or reproductive effects, are often scattered and fragmentary, which can necessitate a more qualitative (i.e., yes or no) evaluation. Such evaluations lend themselves nicely to the use of qualitative structure analyses where the presence of a particular substructure and/or function group is correlated with a specific toxicological endpoint.

Although relationships between chemical structure and biological activity were noted as early as the 1860's, work by Hammett in the 1930's, Taft in the 1950's and Hansch in the 1960's, provided the cornerstones on which QSAR methodologies in the United States have been built for the past 20 years. A number of QSARs are available to estimate a variety of physicochemical endpoints. While they vary in accuracy, especially when dealing with structurally complex molecules, they are, by and large, of good quality. Because of the general lack of both human health and environmental effects data, predictions based on QSARs have in recent years played an ever more important role in the acquisition of these data.

There are a variety of published methods for both qualitative and quantitative estimation of toxicological endpoints. The specific methods used in this model are discussed in Chapter 3 and Appendix A of this report. The quality and amount of data on which these relationships are based is typically less than for physicochemical properties. Therefore, the accuracy of such predicted values varies markedly. Good predictions can be attained, however, for many endpoints, especially effects in the aquatic environment. Structure analysis techniques have not yet been developed for all toxicological endpoints. Moreover, some existing techniques have yet to be validated and/or are limited to a narrow range of chemicals. Whenever used, the limitations of these procedures with respect to accuracy should be kept in mind.

CHEMICALS SELECTED FOR EVALUATION

When this model was developed, 158 chemicals were selected for evaluation, 140 from the 1989 TRI and 21 high-volume pesticides (3 of the pesticides happened to be already included in the chemicals selected from the TRI). The method of choosing which of the more than 270 chemicals in the 1989 TRI to use for development of the algorithm was based on the quantities released. This selection of chemicals based on release and transfer quantities could be considered a preliminary screening tier. The 21 pesticides were selected from annual usage

estimates of the largest volume conventional pesticides in the United States, prepared by EPA (EPA, 1988b; Aspelin, et al., 1992). Appendix B presents a list of all TRI chemicals and indicates which were selected for this evaluation. Appendix B also lists the high-volume pesticides that were selected.

The 1989 TRI gives chemical release and transfer quantities in the categories: 1) fugitive, or non-point, air emissions, 2) stack, or point, air emissions, 3) water discharges, 4) land releases, 5) underground injection releases, 6) transfers to publicly owned treatment works (POTW), and 7) transfers to other off-site locations. In each of these seven categories, in descending order based upon the amount released or transferred in each mode, the pounds released or transferred were summed until enough chemicals had been added up to give 99 percent of the total releases or transfers reported. The chemicals in this 99 percent group became part of the study group; those that contributed to the last one percent of releases were set aside for study at another time.

This procedure was done for all seven categories as well as for total releases and transfers. Any chemical that was part of the 99 percent of releases or off-site transfers in any category was selected. Some chemicals obviously qualified in several categories, but such multiple selection was not used to bias the further evaluation of any compound.

INORGANIC CHEMICALS

It is intended that the algorithm be suitable for use with a wide variety of chemicals, including inorganic chemicals. Inorganic chemicals, however, present unique problems, both from the method used to report inorganics in the TRI and from the limitations of methods available for estimating toxicity or exposure values.

First, several categories of inorganic chemicals are reported in the TRI as "compounds" (i.e., antimony, arsenic, barium, cadmium, chromium, cobalt, copper, manganese, nickel, and lead compounds) for which the specific chemicals released were not reported. The ranking and scoring model depends, however, on specific toxicological information for specific chemical compounds. Therefore, an attempt was made to choose surrogate compounds that represent the most widely used forms of the inorganic chemical categories for evaluation. If the TRI indicated that the majority of the site releases were from a specific industry or application, surrogate compounds that are the major production form of the chemical used in that industry (e.g., arsenic pentoxide for the wood preserving industry) were selected. For cadmium, chromium, nickel and lead, however, no single surrogate was obvious. In these cases, expert judgment was used to select the inorganic salts produced in the greatest quantity. Table 1 lists the inorganic chemicals and chemical surrogates included in the model.

Second, some of the toxicity and exposure data are calculated using QSARs based on 1-octanol-water partitioning coefficients (K_{ow}). The inorganics were considered poorly fat-soluble, which resulted in a lack of reliable methods for calculating missing data. Because many of the ions involved have specific toxic properties, they had to be individually evaluated. Thus, a more extensive literature review was performed to find published experimental data for the inorganics. If data were still unavailable, the missing data were estimated using an SAR. If no SAR was available, the missing datum was flagged and no hazard value was assigned to the missing endpoint.

TABLE 1: TRI INORGANIC CHEMICALS AND SURROGATE COMPOUNDS

TRI Inorganic Compound	Surrogate Compound
Antimony Compounds	Diantimony trioxide (Sb_2O_3)
Arsenic Compounds	Arsenic pentoxide (As_2O_5)
Barium Compounds	Barium chloride ($BaCl_2$)
Cadmium Compounds	Cadmium chloride ($CdCl_2$)
Chromium Compounds	Chromium oxide (CrO_3)
Cobalt Compounds	Cobalt chloride ($CoCl_2$)
Copper Compounds	Copper sulfate ($CuSO_4$)
Lead Compounds	Lead chloride ($PbCl_2$)
Manganese Compounds	Manganese oxide (MnO)
Nickel Compounds	Nickel chloride [a] ($NiCl_2$)
Zinc Compounds	Zinc oxide [b] (ZnO)

(a) To evaluate the mammalian oral toxicity, nickel acetate was the surrogate chosen due to the availability of data.
(b) To evaluate the fish toxicity of zinc compounds, zinc sulfate was the surrogate chosen because zinc oxide is not water soluble.

CHAPTER 3

DEVELOPMENT OF SCORING CRITERIA

Scoring criteria have been divided into three categories: human health effects, environmental effects, and exposure parameters. Table 2 presents the toxicological endpoints included in the model to represent human health and environmental effects. Table 3 lists the environmental effects and exposure parameters used in the model. Each of these scoring criteria are discussed below. Appendix A presents a more detailed description of each of these criteria, including data sources and a description of how the data were scored.

Scoring criteria are divided into three categories: human health effects, environmental effects, and exposure parameters.

HUMAN HEALTH EFFECTS

Human health effects are related to the various toxic responses in humans caused by exposure to a chemical. The screening tier human health effects data included quantitative assessment of acute oral and inhalation toxicity,

Human health effects data include acute oral and inhalation toxicity, carcinogenicity, and "other specific effects."

semiquantitative assessment of carcinogenicity, and qualitative assessment of "other specific effects" (i.e., mutagenic effects, developmental effects, reproductive effects, neurotoxic effects, and other chronic effects). For acute toxicity, rodents were used as surrogate models. In the confirmation tier, evaluation of potency and specific organ/organ system effects could be quantified.

Acute Effects

Acute human health effects can be manifested by a wide range of adverse effects through numerous routes of exposure. Two toxicological endpoints are included in the model to estimate the acute human health

TABLE 2: TOXICOLOGICAL ENDPOINTS

Type of Effect	Type of Toxicity	Toxicological Endpoint
Human Health Effects	Acute	Inhalation LC_{50}[a]
	Acute	Oral LD_{50}[b]
	Chronic	Carcinogenicity[c]
	Chronic	Other Specific Effects[d]
Environmental Effects Terrestrial Animals	Acute	Oral LD_{50}[b]
Fish	Acute	LC_{50}[e]
	Chronic	NOEL[f]

(a) The concentration of a substance in air that will kill half of a group of rodents when inhaled continuously for a specific period of time. Data from tests of eight hours or less were used; these data were scaled on a linear basis to be equivalent to a four hour test by: LC_{50} @4hr = (LC_{50} @*t* hrs)x(*t* hrs)/4 hrs.
(b) The concentration of a substance that will kill half of a group of rodents within 14 days when administered orally as a single dose. (Dose is expressed as mass of chemical per mass of animal body weight.)
(c) Based on the EPA or International Agency for Research on Cancer (IARC) weight-of-evidence classification.
(d) Includes positive evidence of mutagenicity, developmental effects, reproductive effects, other chronic effects and neurotoxicity.
(e) The concentration of a chemical in water that causes death in 50 percent of the fish tested in a 96-hour test.
(f) No observable effect level (NOEL): The highest dosage administered that does not produce toxic effects, estimated from LC_{50} data.

TABLE 3: EXPOSURE PARAMETERS

Persistence	Bioaccumulation
Biological oxygen demand (BOD) half-life[a]	Aquatic bioconcentration factor (BCF)[b]
Hydrolysis half-life[c]	

(a) The number of days required to biodegrade a chemical such that its BOD in water is reduced by half, as predicted using QSAR.
(b) The ratio of the concentration of a chemical in an aquatic organism to its concentration in water.
(c) The number of days required for the amount of a chemical to be reduced by half through hydrolysis in water, at pH 7, as predicted using QSAR.

effects of chemical exposure: oral LD_{50} and inhalation LC_{50}. These endpoints are based on the concentration of a substance that causes death to 50 percent of the exposed population either given a single-dose or continuously exposed to a fixed concentration of a chemical for a short duration. Test protocols for the oral LD_{50} and inhalation LC_{50} have been fairly well standardized and data for these endpoints are often available. The model uses data from laboratory studies of rodents as a surrogate for acute toxicity to humans.

Chronic Effects

Chronic health effects in humans include cancer, mutagenic effects, developmental effects, reproductive effects, neurotoxic effects, and other target organ effects. The carcinogenicity of a chemical based on its weight-of-evidence (WOE) classification was included in the model. Data are generally less available on the other specific chronic effects, but these endpoints were evaluated qualitatively and included in the model.

Carcinogenicity. Carcinogenic effects are observed as tumors (i.e., neoplasms) induced in an organism by exposure to a chemical, via a genotoxic or epigenic mechanism. Several schemes have been developed to classify chemical carcinogens based on the WOE of carcinogenicity. WOE classifications refer only to the amount and adequacy of the available evidence and not to the potency of the carcinogenic effect or the mechanisms involved. Potency refers to the dose required to elicit a toxic effect, in the case of carcinogens, tumors.

The model ranks the carcinogenicity of a chemical using the WOE classification assigned by EPA or IARC. These WOE classifications were available for 48 of the chemicals. For the remaining chemicals, SARs were used to assign carcinogenic effects scores. Potency ofcarcinogenic effects would be included in the confirmation tier.

Other Specific Effects. Other specific human health effects included in the model are mutagenic effects, developmental effects, reproductive effects, neurotoxicity, and other chronic effects. Positive data for mutagenicity is often suggestive of carcinogenicity potential via a genotoxic mechanism. In this assessment scheme, however, it is considered a separate health effect. Mutagenic effects are observed alterations in the genetic material of the germ and/or somatic cells induced by chemical exposure. These alterations may take the form of a gene-loci or point mutation or a clastogenic event (i.e., rearrangements, gains or losses of parts of or whole chromosomes). Since there are few known human mutagens, the correlation between the effects of a chemical on the various mutagenicity test systems and its potential mutagenicity in humans is very difficult to assess. It has been assumed, however, that experimental data even from *in vitro* test systems is an indicator of mutagenic risk to humans.

Developmental effects (e.g., teratogenic and other embryotoxic effects) are observed as damage to the embryo or fetus induced by chemical exposure. Embryotoxic effects include malformation, death and growth retardation. Whole-mammal data is limited but there is evidence for correlation between effects in humans and other mammals. It has been assumed that animal teratogenicity studies are good indicators of human developmental risk. *In vitro* teratogenicity tests appear to be valid for direct acting teratogens. Teratogens requiring metabolic activation, however, are often missed as false negatives.

There are adverse effects of chemical exposure on other aspects of reproduction. These include but are not limited to effects on fertility, gestation and lactation. It has been assumed that adverse reproductive effects in animal studies are good indicators of human risk for like effects. Due to the nature of the endpoints for reproductive effects, *in vitro* tests have not been considered.

Neurotoxic effects are adverse effects on the nervous system induced by exposure to a chemical. These include effects that are structural and/or functional in nature as well as behavioral alterations and learning disabilities. The other chronic effects are the adverse structural, physiological or biochemical effects on various non-reproductive organ systems. Of particular interest are effects on the immune system. Immunotoxic effects are adverse effects on the immune system which include allergic sensitization. These endpoints in general are poorly defined and test systems, both *in vivo* and *in vitro*, are not well documented or well accepted.

Data on the other specific effect endpoints, when available, are difficult to interpret. Furthermore, structure analysis reported for some of the specific effects is limited to certain chemical classes. Despite the limitations of the data, each of these endpoints (e.g., mutagenicity, developmental effects, reproductive effects, neurotoxic effects, and other chronic effects) was evaluated qualitatively (i.e., assigned a "yes" for positive test results or a "no" for negative test results or a lack of data) and combined into one endpoint in the model. Expansion and quantification of this criteria should be performed in the confirmation tier of the human health effects assessment.

ENVIRONMENTAL EFFECTS

Environmental effects are related to the response of populations of organisms representing different trophic levels and different environments exposed to a chemical. As with human health effects, environmental effects data fall into a number of areas. Environmental effects included in the model were quantitative assessment of mammal and fish mortality (fauna representing terrestrial and aquatic environments, respectively), and the aquatic subchronic endpoint of no observable effect in fish. These are effects for which the most experimental data are available and SARs have been the most widely demonstrated. In the confirmation tier, this could be expanded to include responses for flora and species representing different trophic levels.

Environmental effects include acute mammal and fish mortality and chronic sublethal effects in fish.

Terrestrial Effects

Terrestrial effects include toxic effects to various components of the terrestrial environment, including effects on mammals, birds and higher plants. Rodent acute oral toxicity (LD_{50}) serves in the model as a surrogate for terrestrial effects. This endpoint was also used as a surrogate for human acute oral toxicity. At the confirmation tier, bird acute toxicity and higher plant phytotoxicity could be added.

Aquatic Effects

Aquatic effects include toxicity to aquatic organisms exposed to chemicals. Acute fish mortality data (i.e., LC_{50}) is one of the most readily available endpoints and one that can be estimated well by QSARs. The universality of this endpoint makes it important in the screening phase of an evaluation. Fish LC_{50} was selected as a scoring criterion for the screening tier model. Several trophic levels and levels of biological complexity, including microorganisms, algae and invertebrates, could be included in the confirmation tier.

Chronic effects on fish are sublethal effects, typically of longer term exposure and typically measured as the "no observable effect level" (NOEL). The NOEL is defined as the highest dosage administered that does not produce toxic effects. The most sensitive effects are observed in reproduction and growth. The NOEL for many fish has not been measured, but can be

estimated from the acute toxicity data (i.e., the lethal dose to 50 percent of the population) and the octanol-water partition coefficient of the chemical.

EXPOSURE PARAMETERS

Travis and co-workers have defined exposure as the concentration of a chemical in space and time at the interface with a target population (Travis et al., 1983). A chemical once released into the environment is subjected to a variety of physical, chemical and biological processes. These processes are relevant to the amount and distribution of the chemical in the different compartments of the environment and, therefore, affect potential levels and routes of exposure. Processes such as bioaccumulation and persistence, including abiotic (i.e., photolysis and hydrolysis) and biotic degradation (i.e., microbial transformation), are important components of exposure assessment since each has the potential of affecting exposure levels. The amount of chemical released to the environment, the environmental medium of release (e.g., air, water) and local environmental conditions will also obviously affect the potential levels and routes of exposure.

The screening tier exposure assessment includes persistence and bioaccumulation along with annual TRI releases as an overall measure of potential exposure.

The screening tier exposure assessment data includes quantification of persistence (i.e., biotic and abiotic degradation) and bioaccumulation (i.e., aquatic BCF). These exposure criteria are used in the algorithm with the quantity of releases reported in the TRI as an overall measure of potential exposure. Physicochemical properties, such as the 1-octanol-water partition coefficient (K_{ow}), are used indirectly in the model to estimate exposure.

It should be noted that the purpose of this ranking scheme is to address environmental releases and subsequent exposures, thus the emphasis on persistence and bioaccumulation. If the model were applied to the workplace, these factors would be less important to the potential for occupational exposure.

A pivotal aspect of exposure assessment is the use of fate and transport models to quantify the concentration of a chemical as it moves from a source, through the environment, to the target population. Several multi-media fate models have been developed to predict the distribution of a chemical in the environment. The majority of non-site-specific fate and transport models have been based on the concept of fugacity (Mackay, 1979). Fugacity models work by converting chemical concentrations in the major environmental compartments (i.e., air, water, soil, etc.) to fugacity, a thermodynamic equilibrium criterion which has units of pressure. This method of calculation can be extended to a variety of environmental media and has the advantage of being easy to compile and manipulate. Fugacity models have been developed to reflect several levels of complexity. In the confirmation tier, a prediction of the environmental distribution of the pollutant based on fugacity could be included as a further refinement of potential exposure. Site-specific exposure assessments with more tailored chemical fate and transport modeling could also be performed for specific areas of interest, as are done for site-specific risk assessments.

Persistence

Abiotic and biotic transformations/ degradations of a chemical affect its persistence and concentration in the environment. Transformation results in a modification of the parent chemical and the subsequent formation of an analogous or homologous derivative. Degradation is the breakdown of the chemical to water, carbon dioxide, ammonia and other micromolecules. Chemical processes influence

the amount of the chemical present in the environment by regulating abiotic transformations and degradations. Abiotic alteration is primarily a result of the action of light (photolysis), or the reaction of the chemical with water (hydrolysis). Biological processes also influence the concentration and distribution of the chemical in the environment. Biotransformation/biodegradation is a result primarily of microbial action. All of these processes act to reduce the persistence of a chemical in the environment.

Parameters used to measure persistence in the model are BOD half-life and hydrolysis half-life. In general, BOD is the amount of oxygen required by bacteria to reduce the organic matter in water from a waste, typically measured in a 5-day test. In this study, BOD half-life was used as a measure of the number of days required to reduce the BOD from a chemical in water by half due to biodegradation of the chemical. Hydrolysis half-life is the time required to reduce the amount of a chemical in water by half through hydrolysis reaction. Both BOD half-life and hydrolysis half-life were estimated using QSARs due to the wide variability in experimental data. Photolysis half-life is another important measure of persistence but was not included in the model due to a lack of data and of a reliable QSAR to estimate missing data.

The confirmation tier could include an evaluation of other measures of persistence that might be included in the model. Another issue is whether the BOD half-life and hydrolysis half-life criteria (assuming the medium is water) are preemptive and should be combined into one score. If either of these criteria are very short, it is likely that the other criterion could be neglected.

Bioaccumulation

The term bioaccumulation is used to describe the phenomenon by which a chemical is taken up by an organism to a concentration greater than in the surrounding environment. When a chemical accumulates in an organism to a high steady-state level, bioconcentration has occurred. This is a result of the uptake rate constant being larger than the elimination rate constant. In contrast, biomagnification results when oral uptake of a chemical leads to an increase in its concentration from one link to the next in a food chain. BCF is the ratio of the concentration of a chemical in an organism to its concentration in the test medium or environment, typically water, at steady-state conditions. This factor is a measure of the chemical's ability to bioaccumulate and is typically reported in log units.

Bioaccumulation is a function of the physicochemical properties of a chemical, especially the chemical's lipid solubility. The K_{ow} (described below) is commonly used as an estimate of fat solubility. K_{ow} is, in turn, used to estimate BCF. The estimation of the BCF from its relationship with K_{ow} appears to be accurate but varies in formulation depending on the test system (Veith et al., 1983; Geyer et al., 1991). Such estimation may be considered reliable unless metabolic processes are significant.

While bioaccumulation may occur in both aquatic and terrestrial organisms most of the data relates to the former. Bioaccumulation in terrestrial species does not correlate well with bioconcentration in aquatic species because it is not as dependent on chemical lipid solubility. Rather it depends more on the rate of metabolism and other excretion mechanisms.

In aquatic food chains, biomagnification is not a significant aspect of bioaccumulation unless the K_{ow} is greater than 1,000,000 (log K_{ow} greater than 6). The direct bioconcentration of a chemical is often lower than predicted from the K_{ow} and bioconcentration tends to decrease with increasing K_{ow} beyond a log K_{ow} of 6 due to increasing molecular size (Bintein et al., 1993). The use of K_{ow} alone as an estimation of

bioconcentration is limited to un-ionized organic chemicals. Chemicals which dissociate 50 percent or more bioconcentrate significantly less than predicted by K_{ow}-based estimation methods. When evaluating an ionized chemical, consideration should be given to the dissociation constant. These limitations were not considered too significant for purposes of the screening tier, and bioaccumulation, as it pertains to aquatic ecosystems using the BCF, was incorporated in the model.

Physicochemical Properties

The partitioning of a chemical in and between environmental compartments (i.e., air, soil and water) is governed by physicochemical properties such as water solubility, water/organic matter partitioning, vapor pressure, acid dissociation, and soil/sediment adsorption. In addition, physicochemical properties are often used as surrogates for human health and environmental effects. Several of these properties, described below, are used in the model.

Molecular Weight. Molecular weights can be calculated directly from the molecular formula. The major value in having this datum is that it is used for conversion between mass-based (mg/kg or mg/l) and molar-based (moles/kg or moles/l) properties.

1-Octanol/Water Partition Coefficient. The 1-octanol/water partition coefficient, or K_{ow}, is defined as the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase 1-octanol/water system at equilibrium. It is typically reported in log units and is a pivotal parameter in the investigation of environmental fate, representing the distribution tendency of organic chemicals between organic and aqueous phases. It is the most often used single parameter in toxicity QSARs.

K_{ow} is related to lipophilicity (fat solubility), water solubility, soil/sediment adsorption and aquatic BCF. A chemical with a low K_{ow} value is considered hydrophilic and tends to have a low fat solubility, high water solubility, small soil/sediment adsorption coefficient and a small BCF. The converse is also true. The universality of K_{ow} as a descriptor stems from the fact that in reality it is a multicomposite parameter representing a mixture of a wide variety of molecular interactions (Dearden, 1990).

K_{ow} values can be determined experimentally by several methods including the standard shaker flask method and the more novel slow stir method. In addition, several good estimation methodologies exist. The fragment constant method (Rekker, 1977; Hansch and Leo, 1979) has been used to calculate K_{ow} from substitute constants. Constants have been tabulated for approximately a hundred molecular fragments. The MedChem CLOGP software estimates K_{ow} values from an algorithm developed from fragment constants and structural factors. Other K_{ow} estimation schemes include those used in the studies of Ghose and Crippen (1986).

K_{ow} is a key input variable to the QSARs used in this model to predict aquatic acute and chronic toxicity, BOD half-life, and BCF, when experimental data are not available. Thus, experimental values of K_{ow}, rather than predicted values, were preferred. If experimental values were not available, K_{ow} was predicted using the estimation scheme of Ghose and Crippen (1986). For the pollutants evaluated in this exercise, experimental K_{ow} values parallel the predicted ones suitably (see Figure 1).

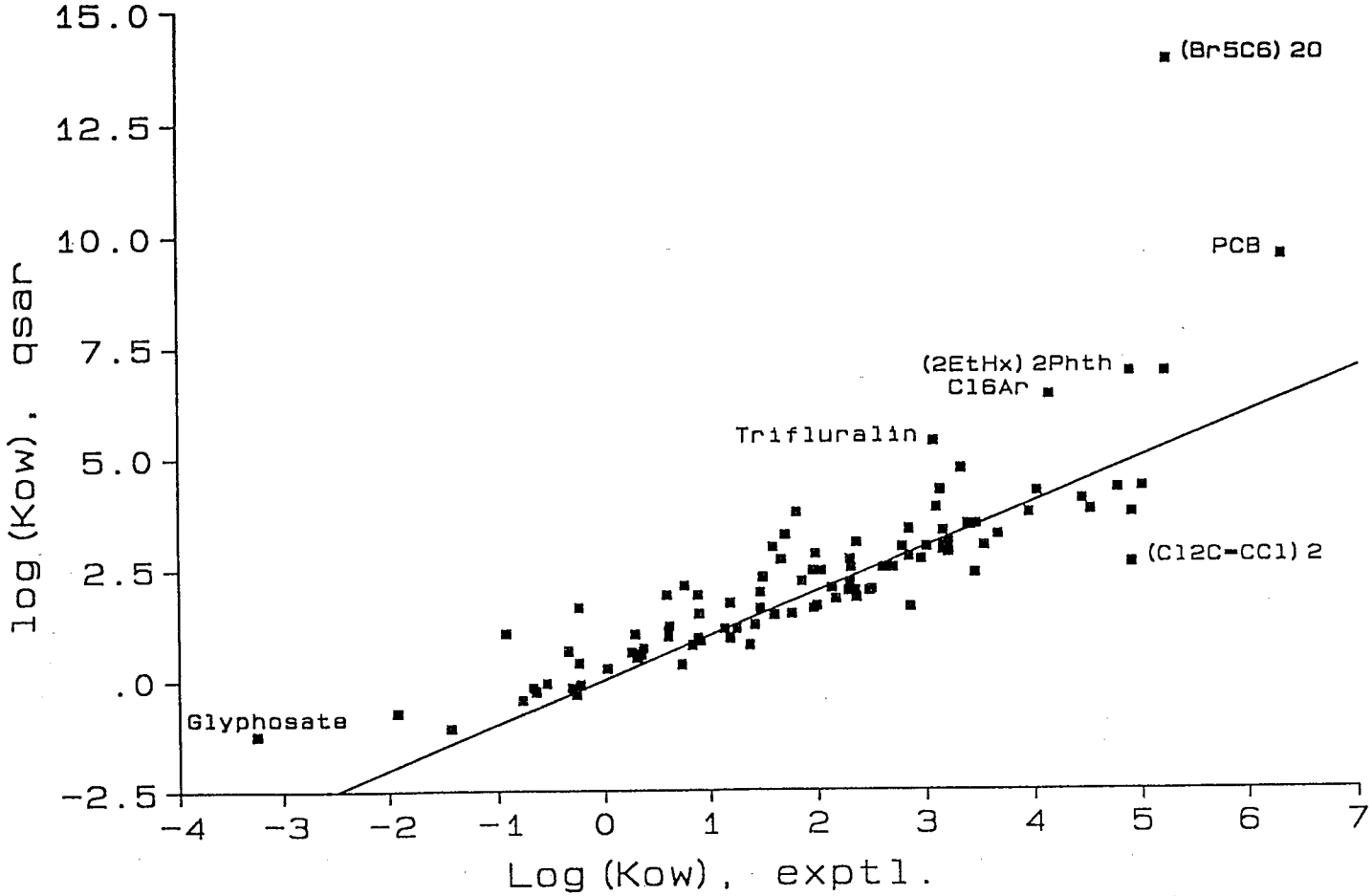

Figure 1. Predicted K_{ow} vs. Experimental K_{ow}

Water Reactivity. Some functional groups, such as acid chlorides, isocyanates, and epoxides react with water in less than one day. If a QSAR or SAR were used to estimate the aquatic environmental effects (i.e., fish LC_{50} and fish NOEL) of such compounds, the effects were assumed to be those of the hydrolysis products which were substituted into the algorithm.

CHAPTER 4

THE ALGORITHM

This chapter presents a description of the algorithm. An exact description of the data sources and scoring of each criteria is included in Appendix A.

The method evaluates the potential hazard of TRI releases to humans, terrestrial animals and fish. A chemical hazard value is calculated based on the toxicity of the chemical, its persistence, and its potential bioaccumulation in the environment.

OVERVIEW

The screening tier chemical ranking method is illustrated conceptually in Figure 2. The method evaluates the potential hazard of TRI releases to humans, terrestrial animals and fish. In the model, a hazard value is calculated for a chemical based on the toxicity of the chemical together with its persistence and potential bioaccumulation in the environment. A weighted hazard value is then calculated that combines the hazard value, based on toxicity, persistence and bioaccumulation, with the weight of nation-wide releases reported in the TRI. The persistence, bioaccumulation and release data are used in the model as a measure of the potential for exposure. The basic algorithm is shown in the box below.

There were several assumptions made in the development of the algorithm. Considering the accuracy of many of the studies of toxicity, it has been assumed that these data are generally only accurate to within an order of magnitude. This allowed some leeway to use QSAR or SAR derived data when experimental data were not available. In this screening-level analysis, the objective in terms of this level of uncertainty was to avoid false negatives. In a more detailed analysis (a later tier), a more thorough search for data could be performed for a smaller number of chemicals.

Basic Algorithm:

Total Hazard Value = (Human Health Effects + Environmental Effects) x Exposure Potential

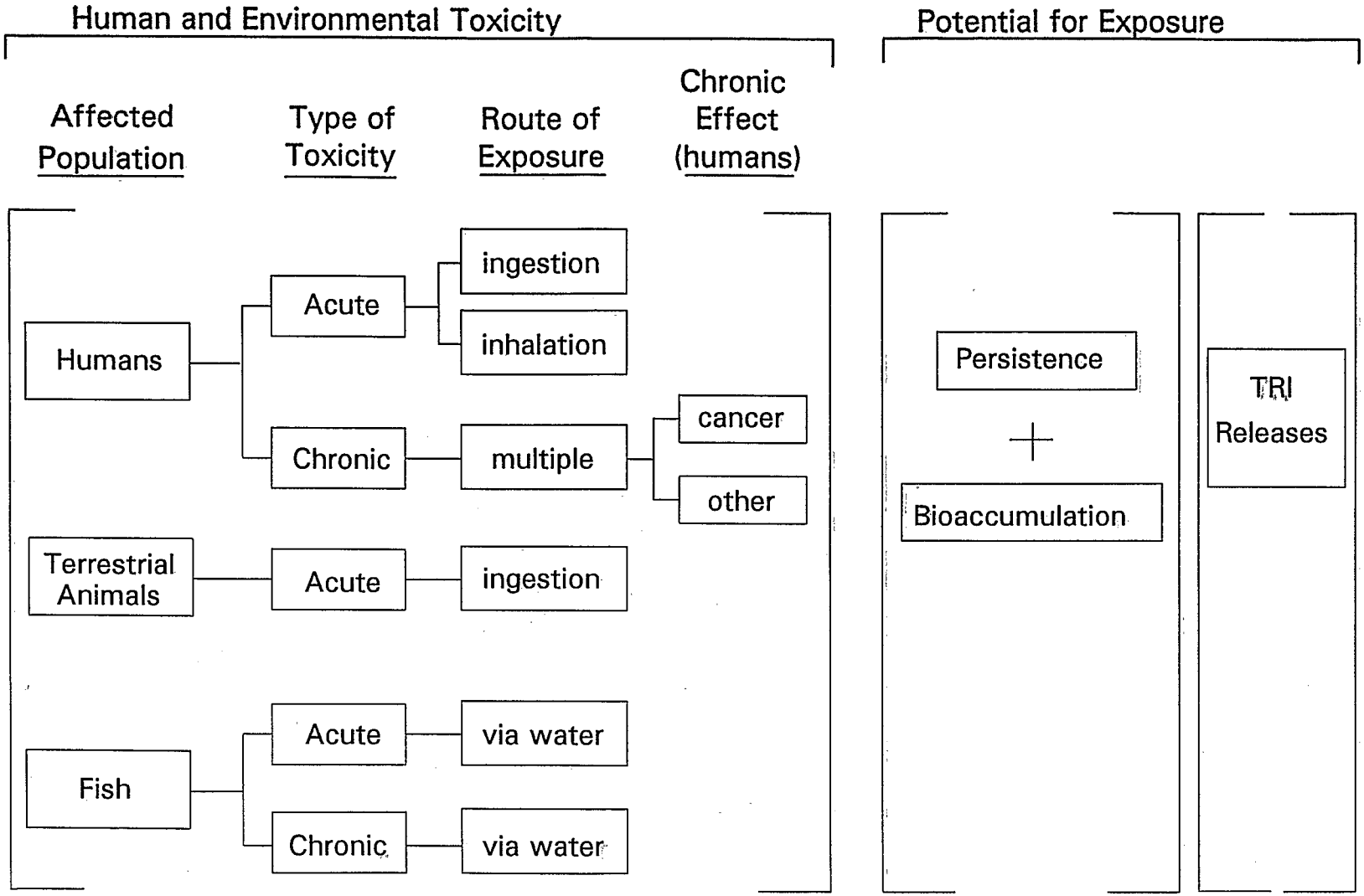

Figure 2. Conceptual Model of Chemical Hazard Ranking Method

Secondly, considering the range of toxicity and physical properties of the pollutants of interest, constructing the algorithm to give an approximate logarithmic response has been deemed appropriate. This allowed pollutants of widely differing properties to be on the same scale. The algorithm, however, does not always adhere to a strict mathematical form for this. For carcinogenicity, for example, the algorithm takes the various WOE classifications assigned by IARC or EPA and specifies a numeric effect rating for each. The net result was an approximate logarithmic (i.e., order of magnitude) scale.

All of the additive terms within this algorithm (i.e., oral LD_{50}, inhalation LC_{50}, carcinogenicity, "other specific effects", fish LC_{50} and fish NOEL) were given equal weighting by assigning a hazard value to each that could range on a scale from zero to five. Cutoff values were chosen for the terms so that the hazard value for very high or very low toxicities would not exceed five or be less than zero, respectively. (See Appendix A for further details of assigning hazard values.) Although the *terms* were weighted equally, there were two aspects that created an implicit weighting of the *endpoints*. First, as previously noted, there were several different kinds of data used as input to the algorithm: quantitative toxicity levels (i.e., LC_{50} and LD_{50}); semi-quantitative levels (i.e., carcinogenicity WOE), and qualitative assignments (i.e., yes/no information on other types of chronic effects). Therefore, assigning hazard values to the group of qualitative chronic effects (e.g., neurotoxicity, mutagenicity) on the same zero to five scale as quantitative toxicity levels for a specific endpoint (e.g., acute inhalation toxicity) gives greater weighting to the one quantitative endpoint than to the group of qualitative effects. Second, the choice of cutoff levels for assigning maximum or minimum hazard values adds a weighted judgment to the algorithm.

Furthermore, the algorithm was to some extent molded by the choice of the chemicals used in the evaluation. The TRI is by its nature a list of toxic chemicals. Of the 112 organics drawn from the TRI, 40 of them, or 35 percent, showed some indication of carcinogenicity. This is higher than the general run of chemicals because selection of chemicals for the TRI, being based on regulatory lists, was affected by carcinogenicity data as well as release amounts.

Each of the toxicological endpoints are treated as additive effects. Persistence and bioaccumulation are considered pivotal to the potential for exposure and are included as multiplicative factors rather than additive effects.

HAZARD VALUE

The hazard value for each chemical is derived from data on the seven toxicological endpoints and the exposure parameters described in Chapter 3. Each of the toxicological endpoints are treated as additive effects. Each additive endpoint receives a hazard value between zero (relatively nontoxic) and five (extremely toxic) based on the results of laboratory tests, carcinogen classification schemes, or QSARs. Although there is implicit weighting involved in assigning hazard values, as discussed above, no additional scalar weighting is currently applied to any toxicological endpoint. The algorithm, however, could be easily modified to do so.

Persistence and bioaccumulation are considered pivotal to the potential for exposure and are included as multiplicative factors rather than additive effects in the algorithm. Each multiplicative criterion is assigned a hazard value between 1 (not persistent or does not

bioaccumulate) and 2.5 (highly persistent or high tendency to bioaccumulate) based on the experimental data or QSARs.

The algorithm is:

Total Hazard Value = (Human Health Effects + Environmental Effects) x Exposure Potential

where:

$$Human\ Health\ Effects = HV_{oral\ LD50} + HV_{inhalation\ LC50} + HV_{carcin} + HV_{other} \quad (max. = 20)$$

$$Environmental\ Effects = HV_{oral\ LD50} + HV_{fish\ LC50} + HV_{fish\ NOEL} \quad (max. = 15)$$

$$Exposure\ Factor = HV_{BOD} + HV_{hydrolysis} + HV_{BCF} \quad (max. = 7.5)$$

and:

HV_x = ***Hazard Value for endpoint x***

Human health effects have the potential of being rated from 0 to 20 (e.g., ten points for acute effects and ten points for chronic effects). Environmental effects have the potential of being rated from 0 to 15. Exposure parameters can be rated from 1 to 7.5 (e.g., up to 2.5 for BOD half-life, hydrolysis half-life and log BCF). Using this scheme, the theoretical maximum total hazard value would be 262.5 (i.e., (20 + 15) * 7.5). The actual maximum for a chemical among those evaluated was 187.5. For 90 percent of the chemicals the total hazard values were below 107. In the algorithm, the final hazard values were normalized to a scale from 0 to 100.

The program has been designed so that the user can change the weightings of each endpoint and determine the effect such a weighting has on the chemical ranking. In this manner, the algorithm may be utilized to obtain a chemical ranking for different purposes. This is discussed further in Chapter 5, where the sensitivity of the algorithm to changes in the endpoint weightings are examined.

CORRELATION OF SCORING CRITERIA

One objective in developing the algorithm was that no one term scored in the algorithm should dominate the results. To determine whether particular terms dominated the total hazard value for the chemicals scored, a linear regression analysis was performed for total hazard value (i.e., the sum of the individual hazard values) versus subtotal hazard value by area (human health, environmental and multiplicative), as well as individual terms and log K_{ow}. The correlation coefficient (r) values from this analysis are reported in Table 4. An r that is neither extremely high nor extremely low, ideally in the range of 0.4 to 0.6 (regardless of sign), would indicate an appropriate level of importance for each term. The results of this regression analysis show that, overall, the model is operating as it should in that no one term dominates the results.

The terms that make up the algorithm should also be independent of each other. Correlations between the some of terms were therefore examined. Because some correlation between carcinogenicity and the "other specific effects" was expected, a linear regression was performed on the hazard values for each term. These results show r = 0.419 for the hazard values for carcinogenicity versus those for "other specific effects", which does not indicate a strong correlation between the two terms.

WEIGHTED HAZARD VALUES

It was planned to use the chemical release and transfer data reported in the TRI together

TABLE 4: SIMPLE CORRELATION COEFFICIENTS (r) FOR FINAL VALUE OF ALGORITHM VERSUS PARAMETER

Parameter	r	Number of Chemicals
log (inhalation LC_{50})	-0.50	121
log (oral LD_{50})	-0.48	158
carcinogenicity	0.43	158
other specific effects	0.37	158
log fish LC_{50}	-0.65	154
log fish no effect	-0.66	154
BOD ½ life	0.32	155
hydrolysis ½ life	-0.06	149
log BCF	0.53	152
all human health terms	0.70	158
all environmental terms	0.76	158
multiplicative exposure factors	0.42	158
log K_{ow}	0.37	158

with chemical production and usage data to calculate weighted hazard values. TRI data are readily available and, although limited to data for certain manufacturing sectors, are the best resource for assessing the overall environmental releases of the chemicals listed. Production and usage data should also provide some measure of the potential releases of a chemical to the environment, particularly for chemicals that are intentionally released, like pesticides and herbicides. Unfortunately, accurate and reliable chemical production and usage data are not available for many of the chemicals listed in the TRI. Thus, surrogates for the total environmental release of a chemical were limited to TRI data, except for pesticides. Since pesticides are designed to be released to the environment, usage data was added to any TRI release data for manufacturing of pesticides to estimate total environmental releases of these chemicals.

Environmental releases of a chemical are obviously pivotal to the potential for exposure, and are thus included as multiplicative factors in the algorithm. Some method of scaling hazard values and release was needed, however, to ensure that neither dominates the algorithm. For example, chemical hazard values calculated by the algorithm can theoretically range from 0 to 262.5 before they are scaled to 100. TRI releases, on the other hand, ranged up to 546 million pounds for ammonium sulfate solution in 1989. Simply multiplying the hazard value by the release would result in a weighted hazard value reflective of the magnitude of the release and not of the toxicity or persistence of the chemical. An option explored in these studies was to weight the hazard value by release data using various schemes.

Weighting schemes examined included:

(1) Multiply the final hazard value by the total releases in pounds (i.e., total releases and transfers reported in the 1989 TRI plus annual usage for pesticides). This approach skews the results almost totally toward the mass of releases.

(2) Multiply the final hazard value by the logarithm of the total releases.

(3) Multiply specific hazard values by the releases to air, to water, or to the sum of air and water.

(4) Multiply specific hazard values by the natural log of the releases to air, water, or the sum of air and water.

The fourth option was selected (see Section A.4 for details). Taking the natural log of the releases provides weighted hazard values that are not dominated by the weight of releases, and does not understate the importance of the release amount. To determine the release amount assigned to air and water categories, the following scheme was applied to the release data. It was assumed that:

- stack and fugitive releases went to air;
- land, injection, water and POTW release went to water;
- annual pesticide usage amounts were assigned to the water release category;
- off-site transfers to an incineration facility were assumed to be destroyed and transfers to a recycling facility were assumed reused and therefore not released to the environment; and
- all other off-site transfers (land, injection, etc.) were assumed released to water. Incineration and recycling amounts were subtracted from total off-site transfers to determine the remainder of off-site transfers released to water.

To determine the weighted hazard values:

- rodent oral LD_{50}, fish LC_{50} and fish NOEL were multiplied by the water releases;
- rodent inhalation LC_{50} was multiplied by the air releases; and
- carcinogenicity and "other specific effects" values were multiplied by the sum of air and water releases.

Applying releases to the type of toxicological endpoint which correlates to the route of exposure adds a slight degree of sophistication to the model that would not be found if all endpoints were simply multiplied by the total release and transfers. The assumptions used to apply releases (e.g., land, injection, water and POTW releases to water, etc.) are simplistic, but they are appropriate considering the level of analysis in this screening tier. This component of the model could be improved in the confirmation tier by incorporation of some type of fate and transport model, such as a fugacity model.

CHAPTER 5

RESULTS AND DISCUSSION

This chapter presents a summary of the results of the algorithm, an analysis of model sensitivity, a discussion of uncertainties and recommendations for future work. The full results are presented in Appendix C and D. For further information concerning the data used for each chemical, contact the University of Tennessee, Center for Clean Products and Clean Technologies.

Different variations of the algorithm were run to examine the effects of release weighting, missing data and the "other specific effects" score on the chemical ranking results. These variations include:

- using or not using chemical release amounts to weight hazard scores;
- using or not using the "other specific effects" score;
- assigning a default hazard value of either zero or five to chemicals with missing data for acute inhalation toxicity, and acute and chronic fish toxicity endpoints; and
- varying the endpoint weighting factors.

It should be noted that although the model provides a numerical ranking of chemicals, the ranking results do not represent any quantitative measure of hazard or risk. In fact, given the uncertainty and variability inherent to the data used to score and rank chemicals, the most appropriate interpretation of the results would be to consider groups of chemicals, i.e., the top 30 chemicals, the top 20 percent, etc., rather than for directly comparing results of one chemical to another.

The model was demonstrated on the selected group of 158 TRI chemicals and high-volume pesticides.

DEMONSTRATION OF THE ALGORITHM

The model was demonstrated on the selected group of 158 TRI chemicals and high-volume pesticides. This demonstration shows that the relative hazards of a large group of chemicals can be scored and ranked on the same scale for the purpose of priority setting. This demonstration also highlights the need for a

confirmation tier as well as the need for expert judgement in performing chemical ranking and scoring.

The top 30 ranked chemicals (approximately the top 20 percent) from release-weighted and unweighted results are presented in Table 5. These results are from the algorithm using a zero hazard value for missing data and including the "other specific effects" score. These results will be considered the baseline for comparison purposes in the sensitivity and uncertainty discussions in the next chapters.

Four general groups of chemicals appear in the top 20 percent: metals, pesticides, mineral acids and ammonia, and other organic compounds. The metals receive high ranking generally because they are persistent, a number are carcinogens and some exhibit high toxicity to fish (e.g., copper). Manganese ranks high despite its relatively low toxicity due to its persistence and high release amounts. The high-ranking pesticides generally are toxic via inhalation and are toxic to fish. 2,4-D also is persistent in the environment.

Mineral acids and ammonia receive high ranking due to both high release amounts and general toxicity. The high ranking of these compounds highlights a problem in the screening tier: they are not expected to be toxic within the pH range found in ambient waters, but the model does not account for any buffering reactions following release to the environment. In fact, many of the acid releases are to deep-well injection where they would be unlikely to contaminate surface water or directly impact aquatic organisms. The other organic compounds (e.g., formaldehyde, styrene) receive high rankings due to various combinations of toxicity, persistence and release amounts.

Table 5 also shows the effect of weighting by chemical releases. Chemicals that rank high in the algorithm when not weighted by releases do so because of toxicity, bioaccumulation and/or persistence, which are chemical-specific properties. Chemicals that are high-ranking when weighted by releases but not otherwise (e.g., ammonia, sulfuric acid) are relatively less toxic, but rank high because of high release amounts.

SENSITIVITY ANALYSIS

Effect of Missing Data

The algorithm was developed to use a database with a complete set of data for each endpoint. For those chemicals missing experimental data, quantitative or qualitative structure-activity relationships (QSARs or SARs) were used to derive an estimate. There were some endpoints, however, where no reliable QSAR or SAR exist to estimate missing data. These were left as missing data. The number of measured, estimated, and missing data points is presented in Table 6. As can be seen, missing data were most significant for the inhalation LC_{50} and "other specific effects" endpoints.

Acute inhalation toxicity was especially problematic; very little data exist for chemicals with low vapor pressures that may nonetheless be acutely toxic as a fume or aerosol. Instead of estimating highly uncertain values, with little ability to relate toxicity to chemical structure, it was decided to assess the sensitivity of the algorithm to the value assigned to this endpoint.

The algorithm was run both with default hazard value scores of zero and five (the minimum and maximum possible values) for each missing data point for the acute inhalation, acute fish and chronic fish toxicological endpoints. The top 30 ranked chemicals from these two variations in the algorithm are presented in Table 7.

TABLE 5: TOP 30 RANKED CHEMICALS FROM ALGORITHM (default HV to zero for missing data)

Rank	Weighted by Releases		Not Weighted by Releases	
1	chromium compounds[a]	(100)[b]	cadmium compounds[a]	(100)
2	arsenic compounds[a]	(99)	arsenic compounds[a]	(82)
3	lead compounds[a]	(95)	terbufos	(81)
4	copper compounds[a]	(87)	hexachloro-1, 3-butadiene[c]	(78)
5	terbufos	(85)	PCB	(71)
6	2,4-D	(85)	trifluralin	(63)
7	nickel compounds[a]	(84)	hexachlorobenzene	(62)
8	formaldehyde	(84)	1,2,4-trichlorobenzene	(62)
9	1,3-dichloropropene	(78)	chromium compounds[a]	(61)
10	trifluralin	(76)	2-nitropropane	(60)
11	cadmium compounds[a]	(75)	formaldehyde	(60)
12	ammonia	(72)	cobalt compounds[a]	(59)
13	sulfuric acid	(72)	lead compounds[a]	(59)
14	hydrogen fluoride	(67)	nickel compounds[a]	(59)
15	nitric acid	(64)	anthracene	(58)
16	hydrochloric acid	(64)	diaminotoluene	(57)
17	styrene	(62)	hydrogen fluoride	(55)
18	chlorpyrifos	(60)	di(2-ethylhexyl)phthalate	(55)
19	hydrogen cyanide	(58)	chlorothalonil	(53)
20	tetrachloroethylene	(58)	2,4-D	(53)
21	trichloroethylene	(56)	1,3-dichloropropene	(52)
22	chlorine	(56)	2,4-dinitrophenol	(52)
23	manganese compounds[a]	(54)	epichlorohydrin	(52)
24	chlorothalonil	(54)	decabromodiphenyl oxide	(51)
25	di(2-ethylhexyl)phthalate	(53)	biphenyl	(51)
26	hexachlorobenzene	(50)	copper compounds[a]	(51)
27	naphthalene	(48)	hydrogen cyanide	(51)
28	phosphoric acid	(48)	styrene	(50)
29	cobalt compounds[a]	(48)	dibutylphthalate	(50)
30	phenol	(47)	2,4-dinitrotoluene	(49)

(a) Table 1 lists the surrogate compounds used for the metal compounds in this evaluation.
(b) Number in parentheses is the total hazard value for that chemical, normalized to a 0 - 100 scale.
(c) Shading indicates a chemical that is unique to one column in the table.

TABLE 6: NUMBER OF MEASURED, ESTIMATED AND MISSING DATA POINTS

Endpoint	Number of Measured Data Points; (% of total)	Number of Estimated Data Points; (% of total)	Number of Missing Data Points; (% of total)
oral LD_{50}	142 (90)	16 (10): SAR	0
inhalation LC_{50}	83 (53)	38 (24): SAR	37 (23)
carcinogenicity	48 (30)	110 (70): SAR	0
other specific effects	115 (73)	0	43 (27)[a]
fish LC_{50}	104 (66)	45 (28): QSAR	4 (3)
fish NOEL	0	154 (97): QSAR[b]	4 (3)
BOD half-life	0	133 (84): QSAR	2 (1)
hydrolysis half-life	0	139 (88): QSAR	1 (0.6)
BCF	8 (4)[c]	142 (90): QSAR	5 (3)

(a) Source of data for "other specific effects" only includes positive test results. Missing data could either be due to negative results or lack of experimental data.
(b) Quantitative values based on the QSARs or experimental data for fish LC_{50}.
(c) Measured data points used for inorganic chemicals only.

From Table 7, it can be seen that six chemicals within the top 30 differ from the algorithm variation with a default hazard value of zero for missing data to the variation with a default hazard value of five. The top 11 ranked chemicals are the same for both variations, with only small differences in relative rank, indicating that the missing inhalation LC_{50} data for the top-ranked chemicals (chromium, lead, arsenic, copper and nickel compounds, and 2,4-D) make essentially no difference in the results for these chemicals.

The missing fish LC_{50} and fish NOEL data do impact the results for zinc (fume or dust) and friable asbestos when a maximum hazard value is assumed. This is also the case for missing acute inhalation data for zinc and barium compounds, phosphorus and maneb. For these chemicals, the sensitivity analysis indicates that the missing data points could be important to the overall ranking results and more effort in locating or estimating data for these endpoints may be warranted. In order to avoid possible false negatives, these six chemicals should be considered for any confirmation tier analysis.

Excluding "Other Specific Effects"

Also, the algorithm was run excluding the "other specific effects" score to determine the effect of this endpoint on the results. This is the only endpoint where an attempt was not

TABLE 7: TOP 30 RANKED CHEMICALS FROM ALGORITHM, SENSITIVITY ANALYSIS FOR MISSING DATA (weighted by releases)

Rank	Default HV to 0 for Missing Data	Default HV to 5 for Missing Data	(endpoint)
1	chromium compounds[a]	chromium compounds[a]	(inhal. LC_{50})[b]
2	arsenic compounds[a]	lead compounds[a]	(inhal. LC_{50})
3	lead compounds[a]	arsenic compounds[a]	(inhal. LC_{50})
4	copper compounds[a]	copper compounds[a]	(inhal. LC_{50})
5	terbufos	nickel compounds[a]	(inhal. LC_{50})
6	2,4-D	2,4-D	(inhal. LC_{50})
7	nickel compounds[a]	terbufos	
8	formaldehyde	formaldehyde	
9	1,3-dichloropropene	1,3-dichloropropene	
10	trifluralin	trifluralin	
11	cadmium	cadmium compounds[a]	
12	ammonia	zinc (fume or dust)[c]	(fish LC_{50}, fish NOEL)
13	sulfuric acid	ammonia	
14	hydrogen fluoride	sulfuric acid	
15	nitric acid	manganese compounds[a]	(inhal. LC_{50})
16	hydrochloric acid	hydrogen fluoride	
17	styrene	di(2-ethylhexyl)phthalate	(inhal. LC_{50})
18	chlorpyrifos	nitric acid	
19	hydrogen cyanide	hydrochloric acid	
20	tetrachloroethylene	asbestos (friable)	(fish LC_{50}, fish NOEL)
21	trichloroethylene	chlorpyrifos	(inhal. LC_{50})
22	chlorine	zinc compounds[a]	(inhal. LC_{50})
23	manganese compounds[a]	styrene	
24	chlorothalonil	barium compounds[a]	(inhal. LC_{50})
25	di(2-ethylhexyl)phthalate	hydrogen cyanide	
26	hexachlorobenzene	tetrachloroethylene	
27	naphthalene	phosphorus (yellow or white)	(inhal. LC_{50})
28	phosphoric acid	maneb	(inhal. LC_{50})
29	cobalt compounds[a]	trichloroethylene	
30	phenol	chlorine	

(a) Table 1 lists the surrogate compounds used for the metal compounds in this evaluation.
(b) Endpoint included in sensitivity analysis.
(c) Shading indicates a chemical that is unique to one column in the table.

made to obtain data for every chemical. Because only positive results were reported in the data base used for this endpoint (Roadmaps - described in Section A.1.3), it has the effect of penalizing chemicals that have been tested.

The top 30 ranked chemicals from the algorithm both including and excluding "other specific effects" are presented in Table 8. From the table, it can be seen that only three chemicals (nitric acid, manganese and hexachlorobenzene) are ranked in the top 20 percent for the algorithm with the "other specific effects" endpoint included that are not in the top 20 percent with the endpoint excluded. Alachlor, zinc compounds and atrazine are ranked in the top 20 percent with the endpoint excluded and not with the endpoint included. Twenty-seven out of the 30 top-ranked chemicals were the same in both cases, although the actual ranking numbers may have changed slightly.

Effect of Varying the Weighting of Endpoints

As mentioned in Section 4.2, the weight assigned to the endpoints in this algorithm can be varied to assign greater or lesser importance to certain endpoints. For selecting chemicals for safe substitutes analysis, equal weighting was assigned to each endpoint. To examine the sensitivity of the algorithm to changes in the endpoint weighting, the following additional model runs were performed:

- the human carcinogenicity endpoint weight was doubled;
- the human acute oral LD_{50} and inhalation LC_{50} weights were cut in half; and
- the weight assigned to environmental effects endpoints (acute oral LD_{50}, acute fish LC_{50}, and fish NOEL) were cut in half.

These results are presented in Table 9 and Appendix D. Table 9 shows the top 30 ranked chemicals, not weighted by release amounts, for even weighting and for each variation of the algorithm listed above. The biggest difference resulted from doubling the carcinogen endpoint weight; there are five different chemicals in the top 30 as compared to the evenly weighted endpoint results. The other variations have only two or three different chemicals ranked in the top 30. These results indicate that the algorithm is not very sensitive to endpoint weights when changed by a factor of two. Greater changes to the endpoint weights may be appropriate in some cases, depending on the particular purpose for which the algorithm might be used.

UNCERTAINTIES

Uncertainties in the algorithm primarily result from uncertainties in the data base. Because one goal of the screening tier is to avoid false negatives, it is recommended that, in general, chemicals with missing data for any endpoint be considered for the confirmation tier. Some exceptions to this might include:

- if the chemical does not rank near the top of the list even with a default hazard value of five assigned to the missing data for that chemical;
- if there are no reported air releases for chemicals with missing data for acute inhalation toxicity; and
- if the physical/chemical properties of the chemical indicate that it would not pose a hazard in the environment.

Table 10 summarizes the chemicals with missing data.

TABLE 8: TOP 30 RANKED CHEMICALS FROM ALGORITHM, SENSITIVITY ANALYSIS FOR "OTHER SPECIFIC EFFECTS" (weighted by releases)

Rank	Default HV to 0 for Missing Data, "Other Specific Effects" Included	Default HV to 0 for Missing Data, "Other Specific Effects" Excluded
1	chromium compounds[a]	chromium compounds[a]
2	arsenic compounds[a]	arsenic compounds[a]
3	lead compounds[a]	terbufos
4	copper compounds[a]	copper compounds[a]
5	terbufos	1,3-dichloropropene
6	2,4-D	lead compounds[a]
7	nickel compounds[a]	nickel compounds[a]
8	formaldehyde	formaldehyde
9	1,3-dichloropropene	ammonia
10	trifluralin	2,4-D
11	cadmium compounds[a]	sulfuric acid
12	ammonia	cadmium compounds[a]
13	sulfuric acid	nitric acid
14	hydrogen fluoride	trifluralin
15	nitric acid[b]	chlorpyrifos
16	hydrochloric acid	hydrochloric acid
17	styrene	hydrogen cyanide
18	chlorpyrifos	chlorine
19	hydrogen cyanide	hydrogen fluoride
20	tetrachloroethylene	styrene
21	trichloroethylene	phosphoric acid
22	chlorine	chlorothalonil
23	manganese compounds[a]	cobalt compounds[a]
24	chlorothalonil	alachlor
25	di(2-ethylhexyl)phthalate	naphthalene
26	hexachlorobenzene	zinc compounds[a]
27	naphthalene	atrazine
28	phosphoric acid	phenol
29	cobalt compounds[a]	di-2(ethylhexyl)phthalate
30	phenol	tetrachloroethylene

(a) Table 1 lists the surrogate compounds used for the metal compounds in this evaluation.
(b) Shading indicates a chemical that is unique to one column in the table.

Table 9. Top 30 Ranked Chemicals for Various Endpoint Weightings (not weighted by releases)

Rank	Even weighting for all endpoints	Double weighting for carcinogen endpoint	Half weighting for acute human health endpoints	Half weighting for environmental effects endpoints
1	Cadmium compounds[a] (100)[b]	Cadmium compounds (100)	Cadmium compounds (100)	Cadmium compounds (100)
2	Arsenic compounds (82)	Arsenic compounds (87)	Arsenic compounds (83)	Arsenic compounds (85)
3	Terbufos (81)	Polychlorinated biphenyls (74)	Polychlorinated biphenyls (78)	Hexachloro-1,3-butadiene (77)
4	Hexachloro-1,3-butadiene (78)	Hexachloro-1,3-butadiene (71)	Hexachloro-1,3-butadiene (74)	Terbufos (75)
5	Polychlorinated biphenyls (71)	Terbufos (70)	Terbufos (73)	Hexachlorobenzene (68)
6	Trifluralin (63)	Chromium compounds (68)	Lead compounds (65)	Polychlorinated biphenyls (68)
7	Hexachlorobenzene (62)	Nickel compounds (66)	Hexachlorobenzene (64)	Formaldehyde (65)
8	1,2,4-Trichlorobenzene (62)	Hexachlorobenzene (65)	Nickel compounds (63)	Diaminotoluene (63)
9	Chromium compounds (61)	Formaldehyde (63)	Chromium compounds (63)	2-Nitropropane (62)
10	2-Nitropropane (60)	2-Nitropropane (62)	Di(2-ethylhexyl)phthalate (62)	Nickel compounds (62)
11	Formaldehyde (60)	Lead compounds (62)	1,2,4-Trichlorobenzene (61)	Chromium compounds (61)
12	Cobalt compounds (59)	Diaminotoluene (59)	2-Nitropropane (61)	Hydrogen fluoride (61)
13	Lead compounds (59)	Di(2-ethylhexyl)phthalate (57)	Cobalt compounds (61)	Trifluralin (61)
14	Nickel compounds (59)	2,4-D (56)	Trifluralin (60)	Lead compounds (58)
15	Anthracene (58)	Trifluralin (54)	Formaldehyde (59)	Hydrogen cyanide (58)
16	Diaminotoluene (57)	1,2,4-Trichlorobenzene (53)	Anthracene (58)	Epichlorohydrin (57)
17	Hydrogen fluoride (55)	Anthracene (53)	Decabromodiphenyl oxide (57)	1,2,4-Trichlorobenzene (56)
18	Di(2-ethylhexyl)phthalate (55)	2,4-Dinitrotoluene (53)	1,3-Butadiene (55)	2,4-D (56)
19	Chlorothalonil (53)	1,3-Butadiene[c] (53)	2,4-D (55)	Vinyl chloride (54)
20	2,4-D (52)	Epichlorohydrin (52)	Copper compounds (54)	Di(2-ethylhexyl)phthalate (52)
21	1,3-Dichloropropene (52)	1,3-Dichloropropene (52)	Diaminotoluene (54)	Anthracene (52)

Rank	Even weighting for all endpoints	Double weighting for carcinogen endpoint	Half weighting for acute human health endpoints	Half weighting for environmental effects endpoints
22	2,4-Dinitrophenol (52)	Styrene (52)	Styrene (53)	2,4-Dinitrotoluene (51)
23	Epichlorohydrin (52)	Cobalt compounds (51)	1,3-Dichloropropene (53)	Chlorothalonil (50)
24	Decabromodiphenyl oxide (51)	Vinyl chloride (50)	2,4-Dinitrotoluene (52)	Styrene (50)
25	Biphenyl (51)	Tetrachloroethylene (50)	2,4-Dinitrophenol (52)	1,3-Butadiene (50)
26	Copper compounds (51)	Hydrogen fluoride (48)	Dibutyl phthalate (51)	Acrylamide (49)
27	Hydrogen cyanide (51)	N-nitrosodiphenylamine (47)	Chlorothalonil (51)	1,3-Dichloropropene (49)
28	Styrene (50)	Trichloroethylene (46)	Tetrachloroethylene (51)	Cobalt compounds (49)
29	Dibutyl phthalate (50)	Chlorothalonil (46)	Epichlorohydrin (50)	2,4-Dinitrophenol (49)
30	2,4-Dinitrotoluene (50)	Acrylamide (45)	Biphenyl (49)	Biphenyl (49)
Chemicals no longer ranked in the top 30:		Decabromodiphenyl oxide (45)	Hydrogen fluoride (49)	Dibutyl phthalate (45)
		Biphenyl (45)	Hydrogen cyanide (40)	Copper compounds (43)
		Copper compounds (45)		Decabromodiphenyl oxide (41)
		Hydrogen cyanide (44)		
		Dibutyl phthalate (43)		

(a) Table 1 lists the surrogate compounds used for the metal compounds in this evaluation.
(b) Number in parentheses is the total hazard value for that chemical, normalized to a 0 - 100 scale
(c) Shading indicates a chemical that was not within the top 30 for the evenly weighted endpoints

TABLE 10: CHEMICALS WITH MISSING DATA

Endpoint	Chemicals with Missing Data	Comments
oral LD_{50}	No missing data	
inhalation LC_{50}	Alachlor	no reported air releases
	Ammonium nitrate (sol'n)	low volatility[a]
	Ammonium sulfate (sol'n)	low volatility[a]
	Antimony compounds[b]	low volatility[a]
	Arsenic compounds[b]	low volatility[a]
	Barium compounds[b]	low volatility[a]
	Butylate	no reported air releases
	Butyl benzyl phthalate	
	Catechol	
	Chlorpyrifos	no reported air releases
	Chromium compounds[b]	low volatility[a]
	Cobalt compounds[b]	low volatility[a]
	Copper compounds[b]	low volatility[a]
	2,4-D	
	2,4-dinitrophenol	
	2,4-dinitrotoluene	
	Decabromodiphenyloxide	
	Bis (2-ethylhexyl) adipate	
	Di-(2-ethylhexyl) phthalate	high rank for HV=5[c]
	Glyphosate	no reported air releases
	Hydroquinone	
	Lead compounds[b]	low volatility[a]
	Maneb	low volatility[a]
	Manganese compounds[b]	low volatility[a]; high rank for HV=5[c]
	Metolachlor	no reported air releases
	Metribuzin	no reported air releases
	Molybdenum trioxide	low volatility[a]
	Nickel compounds[b]	low volatility[a]
	Nitrobenzene.	
	N-nitrosodiphenylamine	no reported air releases
	Di-n-octylphthalate	
	Phosphorus	
	Picric acid	
	Polychlorinated biphenyls	no reported air releases
	Terephthalic acid	
	Thorium dioxide	low volatility[a]
	Zinc compounds[b]	low volatility[a]
carcinogenicity	No missing data - all chemicals for which EPA/IARC classification not available were examined by SAR	

Table 10, continued

Endpoint	Chemicals with Missing Data	Comments
other specific effects		There are 43 chemicals which received a zero for other specific effects. The data base used, Roadmaps, lists references for positive results only. Some of these chemicals may have been tested, with negative results.
fish LC_{50}	Aluminum (fume or dust) Asbestos (friable) Thorium dioxide Zinc (fume or dust)	high rank when HV=5[c] high rank when HV=5[c]
fish NOEL	Aluminum (fume or dust) Asbestos (friable) Thorium dioxide Zinc (fume or dust)	high rank when HV=5[c] high rank when HV=5[c]
BOD half-life	Maneb Phosphorus	no K_{ow}[d]
hydrolysis half-life	Maneb	no K_{ow}[d]
BCF	Maneb Aluminum (fume or dust) Titanium tetrachloride Thorium dioxide Molybdenum trioxide	no K_{ow}[d]

(a) No experimental data expected due to low volatility of chemical.
(b) Table 1 lists the surrogate compounds used for the metal compounds in this evaluation.
(c) When given a hazard value of five for missing data, this chemical ranks in the top 20 percent.
(d) QSAR could not be run for this chemical due to lack of K_{ow} data.

SELECTION OF PRIORITY CHEMICALS

The chemical ranking and scoring method was developed as a priority-setting tool, to select priority chemicals for evaluating the potential for safe substitutes (Davis, et al., 1994a). Of the top 30 ranked (release-weighted) chemicals identified in Table 5, seven had been selected previously as priority chemicals because they were either included in the EPA 33/50 Program (for voluntary reductions in TRI releases) or manufactured from a 33/50 chemical. These chemicals include chromium compounds, lead compounds, nickel compounds, cadmium compounds, hydrogen cyanide, tetrachloroethylene, trichloroethylene and styrene (manufactured from benzene). Excluding these chemicals from the selection process, the top eight priority chemicals are:

- arsenic compounds
- copper compounds
- terbufos

- 2,4-D
- chlorine
- manganese compounds
- di(2-ethylhexyl)phthalate

Reasons for not selecting some of the other top-ranked chemicals are discussed below.

Terbufos, an insecticide/nematicide, and 2,4-D, an herbicide, were selected to represent the range of top-ranked pesticides. Although some of the other pesticides on the list may be used in different applications (e.g., different crops or pests), many of the safe substitute approaches identified for terbufos and 2,4-D will likely be applicable.

Ammonia and the mineral acids were not selected because the types of releases of these chemicals reported in the TRI probably do not result in exposures to humans or fish to acutely toxic concentrations. It is likely that these chemicals would have a lower ranking in a more sophisticated model that considers the fate of chemicals in the environment. This is not to downplay the possible significance of the effects of large releases or accidental spills of these chemicals. Their high ranking underscores the fact that their toxicity and high release amounts are areas of potential concern.

Copper compounds and manganese compounds were selected for further evaluation. These chemicals, however, point to one of the limitations of the TRI in that it groups metal compounds. No data is provided on the speciation of compounds released to different environmental media, nor on the particular compounds released in the largest amount. The toxicity of metal compounds and their availability to different types of organisms is, of course, highly dependent on the speciation of the compounds. The copper and manganese compound surrogates (copper sulfate, manganese oxide) used in the algorithm are highly to moderately toxic to fish, but other copper or manganese compounds may have lower overall toxicity and would thus rank lower in the model.

The model uses a risk assessment approach to place chemical release data into perspective by combining release amounts with the potential for environmental persistence and bioaccumulation, and potential human health and ecotoxic effects from these releases.

CONCLUSIONS AND RECOMMENDATIONS

The UT chemical ranking and scoring model was found to be a useful tool for screening purposes, and for putting the TRI data in a more useful framework than simply pounds of releases. The model uses a risk assessment approach to place chemical release data into perspective by combining release amounts with the potential for environmental persistence and bioaccumulation, and potential human health and ecotoxic effects from these releases. The model was developed as a tool to select priority chemicals for safer substitutes assessment, and with the concurrent use of expert judgement, it serves as an improvement over previous methods of prioritization. It is also flexible enough for other applications. The UT model has been used to make a preliminary assessment of the comparative potential hazards posed by the reported releases of toxic chemicals in Tennessee, Texas, Louisiana, Indiana and Ohio in 1990, the five states with the greatest releases in that year's TRI (Kincaid and Bartmess, 1993). It is also being modified for use by a major chemical company in prioritizing reduction efforts for TRI releases.

Recommendations for future work include:

- addressing in greater depth the issues resulting from missing data, or considering alternate sources of data;

- further developing the chronic human health effects scoring, for example, by using cancer slope factors and chronic reference doses or other measures of potency rather than semi-qualitative WOE data or qualitative "type of effects" data;

- using the algorithm on a site- or facility-specific basis;

- incorporating chemical fate and transport modeling into the algorithm, i.e., considering the short-term and long-term distribution of chemicals in environmental media, which might include photolysis or other degradation reactions, acid/base buffering reactions, and metals complexation in the environment; and

- developing the second, or confirmation, tier.

Overall, this screening tier should be considered a first step. It should be remembered that this model is a screening tool and was not designed to be removed from expert judgement. In some aspects the model was found to be lacking in sensitivity in that it does not adequately represent chemical behavior in the environment, but it was found to put environmental release data in a more useful framework for priority setting.

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APPENDIX A
DATA SELECTION AND DETERMINATION OF HAZARD VALUES

A.1 HUMAN HEALTH EFFECTS

A.1.1 Acute Effects

Definitions/Test Methods

Oral LD_{50}: The concentration of a substance, expressed in mass of the substance per mass of the animal, that will kill half of a group of rodents within 14 days when administered orally as a single dose.

Inhalation LC_{50}: The concentration of a substance in air (gas or dust) that will kill half of a group of rodents when inhaled continuously for 8 hours or less, scaled to 4 hours.

Data Selection

Figure A-1 shows the hierarchy for Oral LD_{50} data selection. Figure A-2 presents the hierarchy for Inhalation LC_{50} data selection. Experimental data are preferred for both oral and inhalation data. The hierarchy for experimental data sources was 1) Hazardous Substances Data Bank (HSDB, 1993), and 2) Registry of Toxic Effects of Chemical Substances (RTECS, 1992, 1993), both on-line data sources. Additional data sources such as ambient water quality criteria documents were used for the inorganic chemicals (Davidson, et al., 1987; Hose, et al., 1989; IPCS, 1990, IPCS, 1991; EPA, 1980a; EPA, 1980b, EPA, 1980c; EPA, 1980d; EPA, 1980e, EPA, 1984a). Additional data sources were also used for pesticides (Kidd and James, 1991; EPA, 1984b).

If experimental oral LD_{50} data are available for more than one species of rodent, the most sensitive test result is selected. If experimental inhalation data are available for more than one test duration, the datum is selected from the test with duration closest to 4 hours but not exceeding 8 hours.

Since the test durations for the inhalation toxicity tests differ, a linear scaling function was incorporated into the algorithm. The EPA requires a minimum test duration of 4 hours (40 C.F.R. 798.1150). Other test durations were scaled to the 4 hour test by the following equation: $\text{concentration}_1 * \text{time}_1 = \text{concentration}_2 * \text{time}_2$

If experimental data are not available, but can be estimated by way of a structurally similar compound in the same physical state, an SAR is used to estimate the oral or inhalation value. If an SAR is not available, the missing data is flagged in the database and the hazard value for the missing endpoint is set to zero.

Calculation of Hazard Values

Hazard value scores for the inhalation and oral acute toxicological endpoints are based on the $\log_{10}$ of the LC_{50} and LD_{50}. Figure A-3 is a decision tree used to calculate the Oral LD_{50} hazard value.

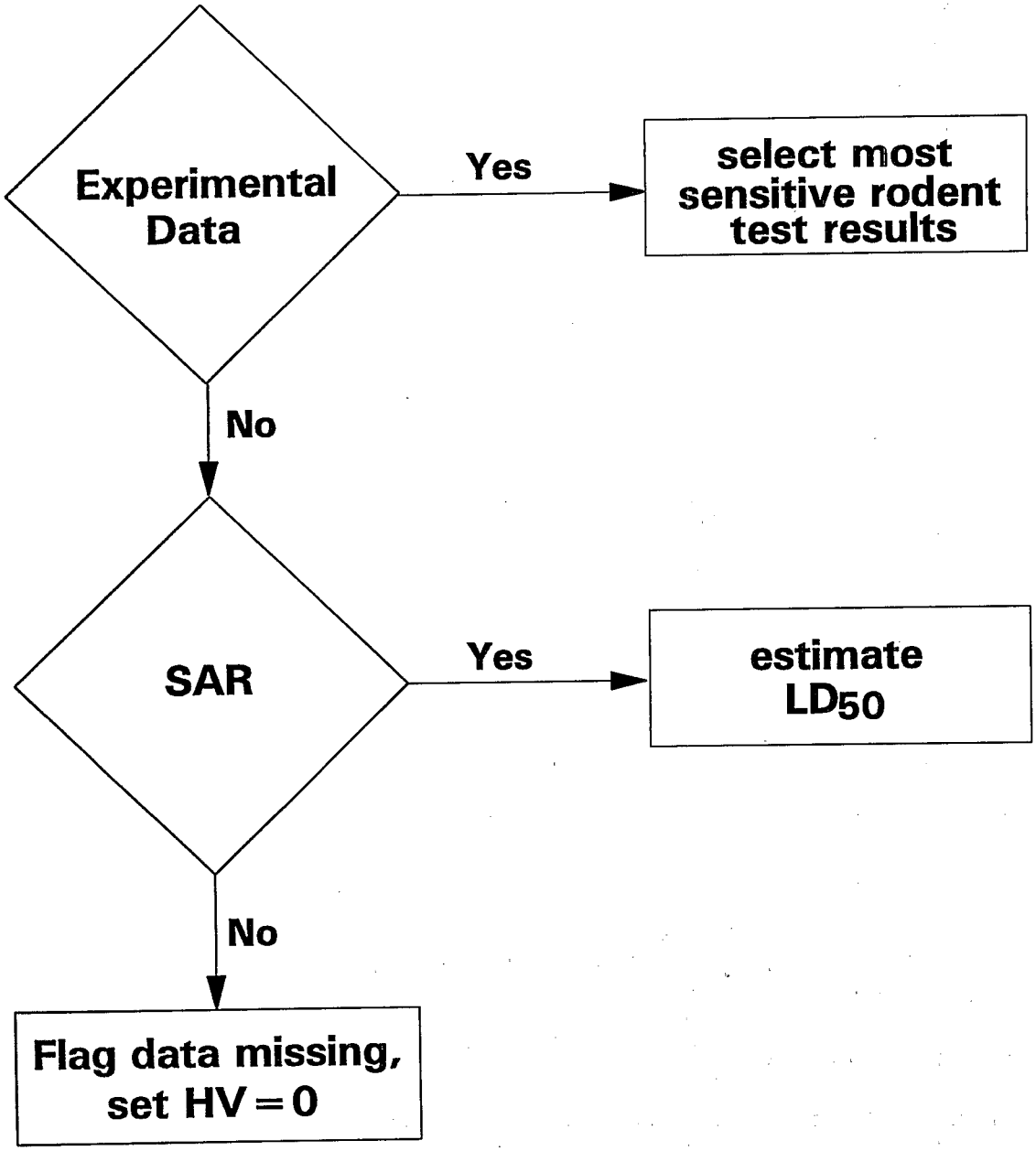


Figure A-1. Decision Tree for Oral LD_{50} Data Selection

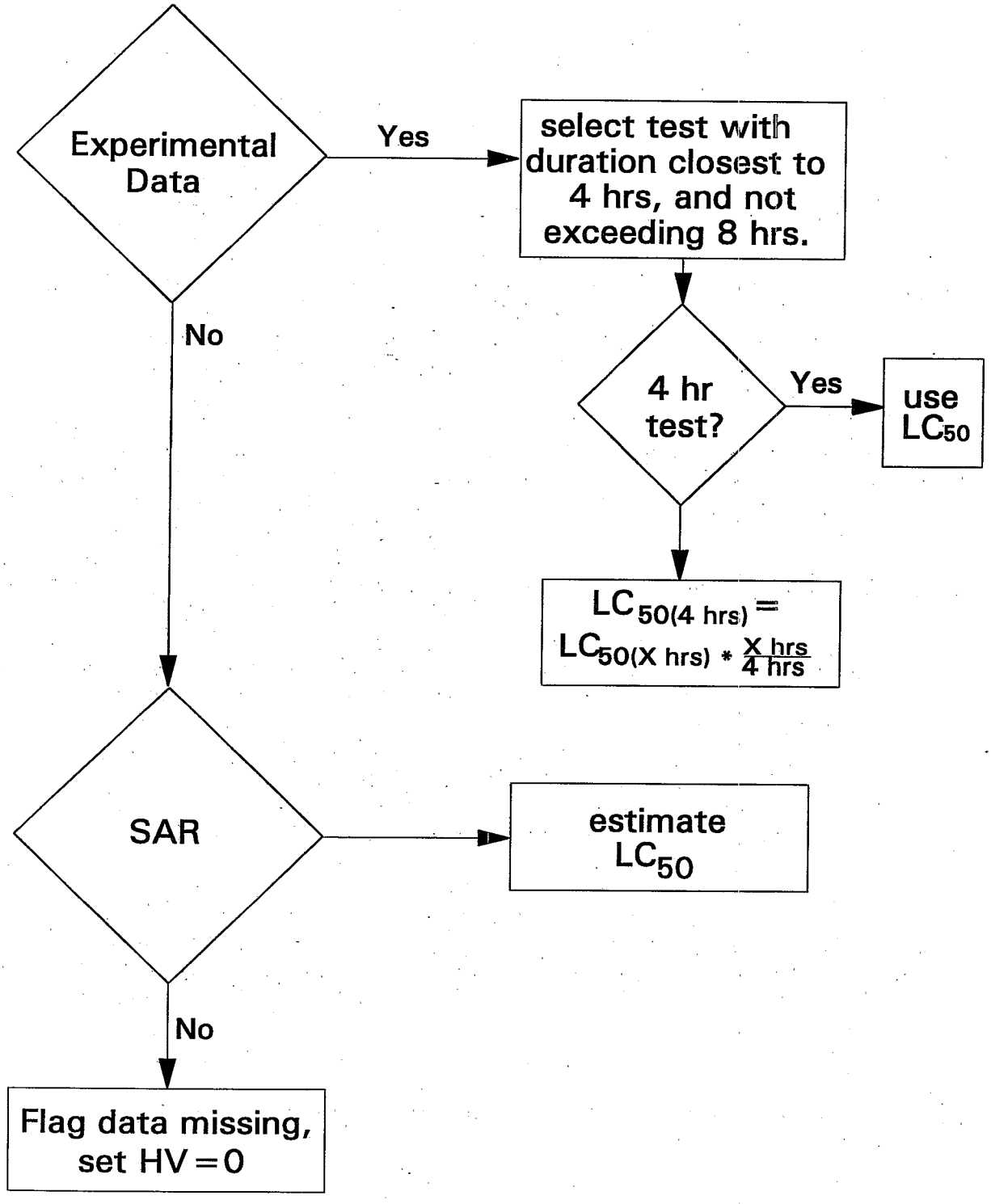


Figure A-2. Decision Tree for Inhalation LC_{50} Data Selection

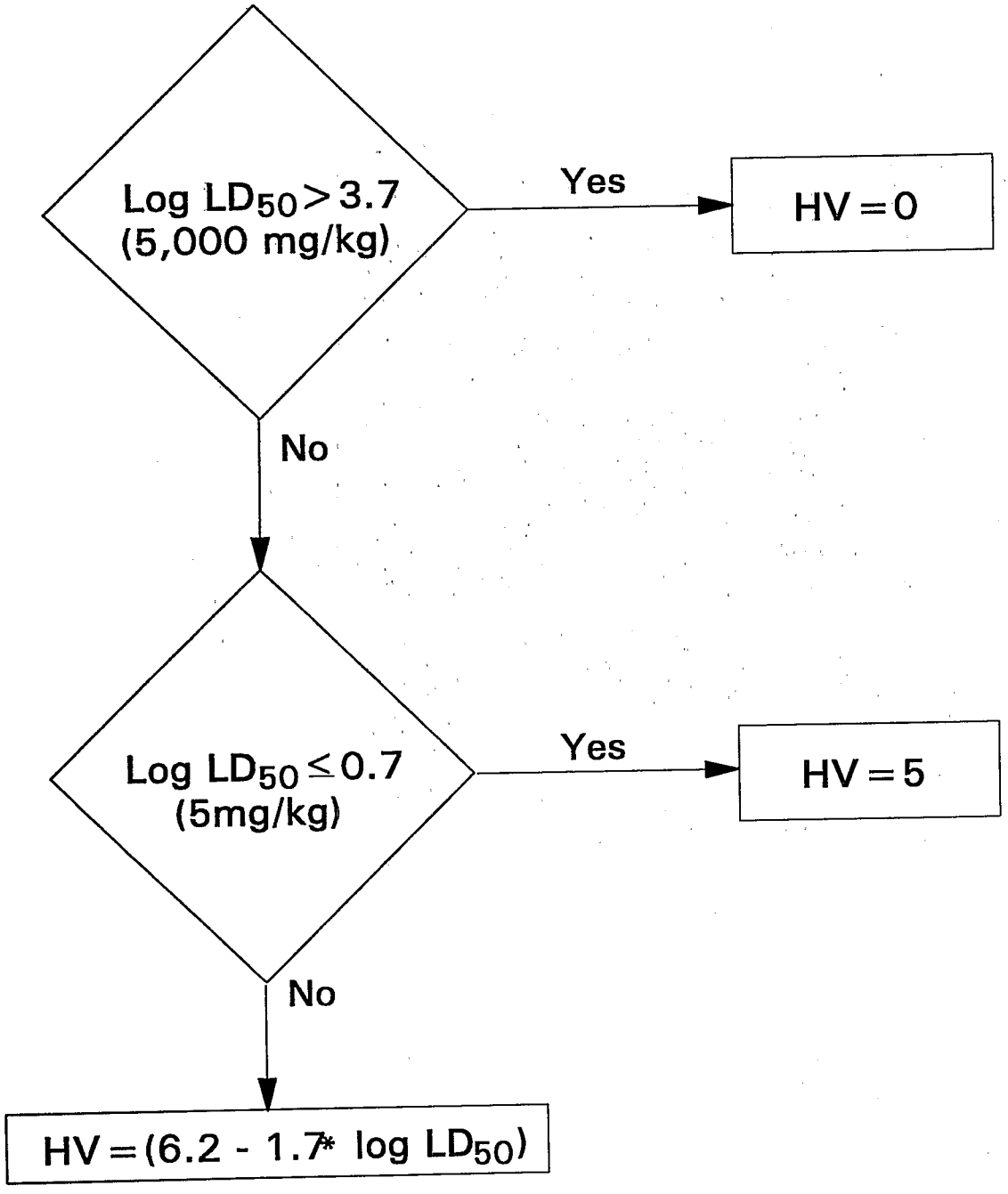


Figure A-3. Decision Tree for Oral LD_{50} Hazard Value

The $\log_{10}$ of the LD_{50} is taken and assigned a score between 0 and 5, using a continuous, linear function. Numerical cutoff values are based on commonly accepted values (Michigan CMR, 1987).

Figure A-4 is a decision tree of the method used to calculate the inhalation LC_{50} hazard value. The $\log_{10}$ of the LC_{50} is taken and assigned a score between 0 and 5, using a continuous, linear function. Numerical cutoff values are based on commonly accepted values (Konemann and Visser, 1988; O'Bryan and Ross, 1988; Weiss, et al., 1988).

A.1.2 Carcinogenicity

Definitions/Classification Methods

IARC Classification: The IARC publishes a series of monographs entitled "IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans," which provide WOE classifications of chemical carcinogenicity. Chemicals are classified by a working group of experts in chemical carcinogenesis and related fields based on published information available at the time the working group was convened. Table A-1 presents the IARC classification scheme.

TABLE A-1: IARC CARCINOGEN CLASSIFICATION SYSTEM

Group	Definition
4	The agent is probably not carcinogenic to humans. - This classification is used when there is *evidence suggesting lack of carcinogenicity* in both humans and experimental animals. (In some circumstances, agents for which there is *inadequate evidence* of or no data on carcinogenicity in humans but *evidence suggesting lack of carcinogenicity* in experimental animals, consistently and strongly supported by a broad range of other relevant data, may be classified in this group.)
3	The agent is not classifiable as to its carcinogenicity to humans. - This classification is used when agents cannot be placed in any other group.
2B	The agent is possibly carcinogenic to humans. - This classification is generally used when there is *limited evidence* in humans in the absence of *sufficient evidence* in experimental animals. (It may also be used when there is *inadequate evidence* of carcinogenicity in humans or when human data are nonexistent but there is *sufficient evidence* of carcinogenicity in experimental animals. In some instances, an agent for which there is inadequate evidence or no data in humans but *limited evidence* of carcinogenicity in experimental animals together with supporting evidence from other relevant data may be placed in this group.)
2A	The agent is probably carcinogenic to humans. - This classification is used when there is *limited evidence* of carcinogenicity in humans and *sufficient evidence* in animals. (Exceptionally, an agent may be classified into this category solely on the basis of *limited evidence* of carcinogenicity in humans or of *sufficient evidence* of carcinogenicity in experimental animals strengthened by supporting evidence from other relevant data.)
1	The agent is carcinogenic to humans. - This classification is used only when there is *sufficient evidence* of carcinogenicity in humans.

source: McGregor, 1992

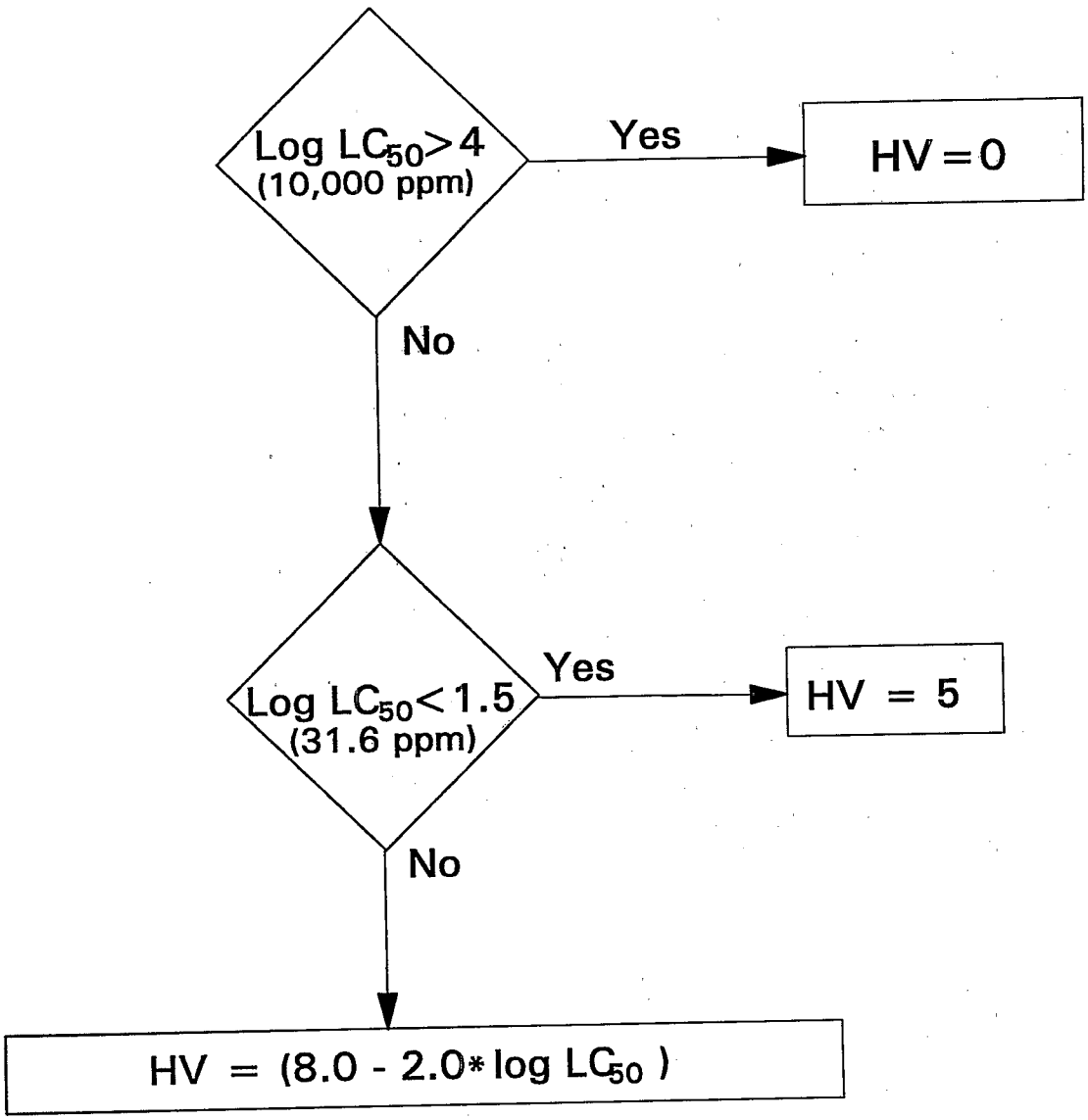


Figure A-4. Decision Tree for Inhalation LC_{50} Hazard Value

EPA Classification: The Carcinogen Assessment Group in EPA's Office of Health and Environmental Assessment prepares WOE classifications for carcinogens. EPA's classification scheme is based largely on an earlier version of the IARC classification scheme which did not include Group 4 and the criteria for Group 2A and 2B. Table A-2 presents the 1986 EPA carcinogen classification scheme. EPA in 1988 began an effort to revise its carcinogen classification scheme (EPA, 1988).

TABLE A-2: 1986 EPA CARCINOGEN CLASSIFICATION SYSTEM

Group	Definition
E	Evidence of Non-Carcinogenicity for Humans. This classification is used when agents show no evidence of carcinogenicity in at least two adequate animal tests in different species or in both adequate epidemiologic and animal studies.
D	Not Classifiable as to Human Carcinogenicity. This classification is generally used when there is inadequate human and animal evidence of carcinogenicity or when no data are available.
C	Possible Human Carcinogen. This classification is used when there is limited evidence of carcinogenicity in animals in the absence of human data.
B	Probable Human Carcinogen. This group is divided into two subgroups, B1 and B2. Subgroup B1 is usually used when there is limited WOE of human carcinogenicity based on epidemiologic studies. Group B2 is used when there is sufficient WOE of carcinogenicity based on animal studies, but inadequate evidence or no data from epidemiologic studies.
A	Human Carcinogen. This classification is used only when there is sufficient evidence from epidemiologic studies to support a causal association between exposure to the agent and cancer.

Data Selection and Calculation of Hazard Value

Figure A-5 is a decision tree of the hierarchy of carcinogenicity data selection. If EPA and IARC have both classified the carcinogenicity of a chemical, both classifications are used to calculate the chemical hazard value. When both IARC and EPA classifications are available for a chemical, the hazard value is assigned for each and the average is taken for the overall hazard value unless the IARC classification is a 3. In this case, only the EPA classification will be used to determine the hazard value. Otherwise, the hazard value is based on the classification available. If neither IARC nor EPA have classified the chemical as a carcinogen, the carcinogenicity of the chemical is evaluated using an SAR in MICROQSAR Version 2.0 which is based on the unpublished work of Arcos. The SAR assigns a positive carcinogenicity rating to a chemical if it contains one or more molecular substructure that has been related to carcinogenicity, such as a polyaromatic hydrocarbon.

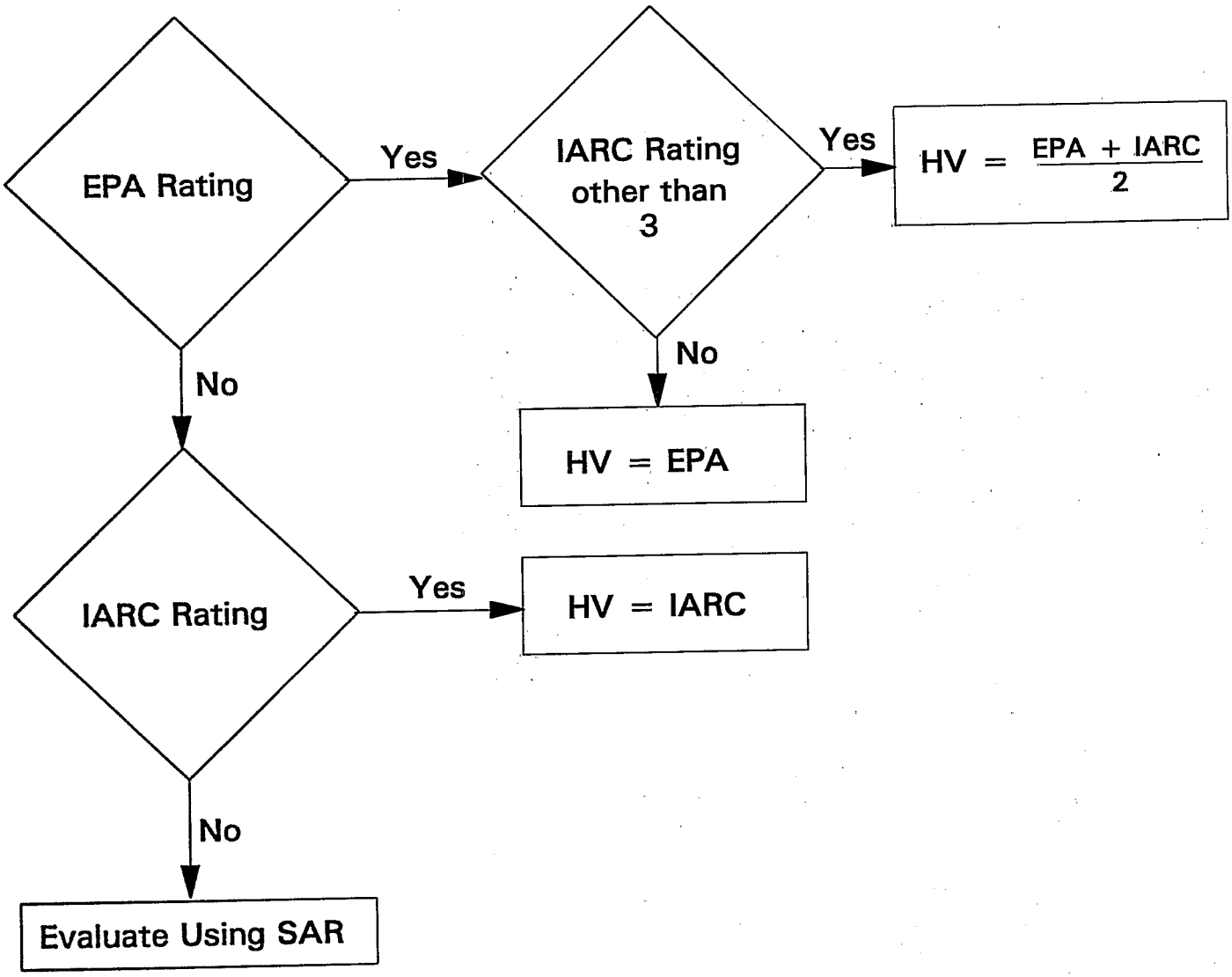


Figure A-5. Decision Tree for Carcinogenicity Hazard Value

Before assigning hazard values to the IARC and EPA carcinogen groups, 31 chemicals for which WOE carcinogenicity ratings had been assigned by both EPA or IARC were reviewed to evaluate the correlation between EPA and IARC ratings. Table A-3 presents a comparison of the EPA and IARC ratings for the 31 chemicals. Based on the definitions provided in the EPA and IARC classification systems, it appears that IARC Group 2A corresponds to EPA Group B2 and IARC Group 2B corresponds to EPA Group B1. Based on actual ratings of chemicals, however, the strongest correlation of IARC Group 2B is seen with EPA Group B2.

TABLE A-3: COMPARISON OF EPA AND IARC RATING OF 31 CARCINOGENS

EPA Rating	IARC Rating	Number of Chemicals
A	1	6
B1	2A	4
B2	2A	2
B2	2B	12
B2	3	2
C	3	5

Thus, EPA Group B2 and IARC Group 2B were assigned equivalent hazard values in the ranking method.

Table A-4 presents the hazard values assigned to IARC and EPA carcinogenicity ratings. Chemicals assumed to be carcinogens based on SARs were assigned a hazard value of 3.0 or 1.0, based on the molecular substructures present.

TABLE A-4: CARCINOGENICITY HAZARD VALUES

IARC Classification		EPA Classification	
Group	Hazard Value	Group	Hazard Value
4	0	E	0
3	0[a]	D	0
N/A	N/A	C	1.5
2B	3.5	B2	3.5
2A	4.0	B1	4.0
1	5.0	A	5.0

(a) The EPA classification alone is used in this case.
N/A = not applicable

A.1.3 Other Specific Effects

Definitions/Test Methods (from Roadmaps):

Mutagenicity: Chemicals are indicated as possible mutagens in humans if positive results in bioassays are reported in the reference source (ICF, 1989).

Developmental Toxicity: Chemicals are indicated as exhibiting developmental toxicity if data in the reference source support concern that the chemical may cause embryotoxicity, fetotoxicity or teratogenicity in humans (ICF, 1989).

Reproductive Toxicity: Chemicals are indicated as exhibiting reproductive effects if data in the reference source support concern that the chemical has adverse effects on male or female reproductive performance (ICF, 1989).

Chronic Toxicity: Chemicals are indicated as exhibiting chronic toxicity if adverse effects other than cancer occur at doses less than or equal to 1 g/kg/day following inhalation, oral or dermal exposure for more than 90 days (ICF, 1989).

Neurotoxicity: Chemicals are indicated as neurotoxic if chronic (at least 90 days) inhalation, oral or dermal exposure to doses less than or equal to 1g/kg/day results in neurotoxic effects (ICF, 1989).

Data Selection and Calculation of Hazard Value

Data for the "other specific effects" endpoints were obtained from Roadmaps, a database developed by EPA of sources of information on the SARA 313 chemicals (ICF, 1989). Roadmaps contains information for the SARA 313 chemicals on health and environmental effects, federal regulations, state air and water regulations and monitoring data, and state contacts. It also summarizes the publicly available toxicity information from a number of data bases. Roadmaps indicates if there was sufficient evidence that exposure to a chemical substance resulted in the indicated health or environmental effect. It indicates that data is available relative to the effect, but it does not report severity or validity of concern, and it does not report numerical test results.

Data in Roadmaps on other specific effects are divided into five categories: 1) chronic toxicity, i.e., health effects (non-cancer) from long-term exposure, 2) developmental toxicity in humans, 3) heritable genetic and chromosomal mutation in humans, 4) neurotoxicity from chronic exposure, and 5) reproductive toxicity. If data are available which imply exposure to a chemical has one of these five toxic effects, Roadmaps flags the endpoint and lists the source of the data. It should be noted if an effect is not flagged for a chemical it does not necessarily indicate negative test results; it could mean either that the available data did not support a concern or that data was unavailable. Table A-5 lists the data sources that Roadmaps references for each of the five endpoints.

TABLE A-5: DATA SOURCES FOR "OTHER SPECIFIC EFFECTS" CITED IN ROADMAPS

Endpoint	Data Sources
Chronic toxicity	DWCD, HAD, HEA, HEED, HEEP, HSDB
Developmental toxicity	ATSDR, DWCD, HAD, HEA, HEEP, HSDB
Mutagenicity	ATSDR, GENETOX
Neurotoxicity	HAD, HEA, HEEP, HSDB
Reproductive toxicity	ATSDR, DWCD, HAD, HEA, HEEP, HSDB

KEY:

ATSDR	Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profile
DWCD	Drinking Water Criteria Documents, EPA
GENETOX	Genetic Toxicity Chemical Information System (on-line database)
HAD	Health Assessment Documents, EPA
HEA	Health Effects Assessment, EPA
HEED	Health and Environmental Effects Documents, EPA
HEEP	Health and Environmental Effects Profiles, EPA
HSDB	Hazardous Substance Data Bank, National Library of Medicine TOXNET (on-line database)

Roadmaps data are incorporated into the chemical hazard ranking method data base. A value of 1 was assigned for each flagged endpoint. If the endpoint was not flagged, a value of 0 was assigned. The values for the five endpoints were summed in "other specific effects", for a maximum of 5 for each pollutant.

A.2 ENVIRONMENTAL EFFECTS

A.2.1 Terrestrial Effects

Definitions/Test Methods:

Oral LD_{50}: The concentration of a substance, expressed in mass of the substance per mass of the animal, that will kill half of a group of rodents within 14 days when administered orally as a single dose.

Data Selection and Calculation of Hazard Value

The rodent oral LD_{50} data used for the acute human health effect endpoint was also used as a surrogate to represent terrestrial organisms. The hazard values are assigned like those for acute human health effects.

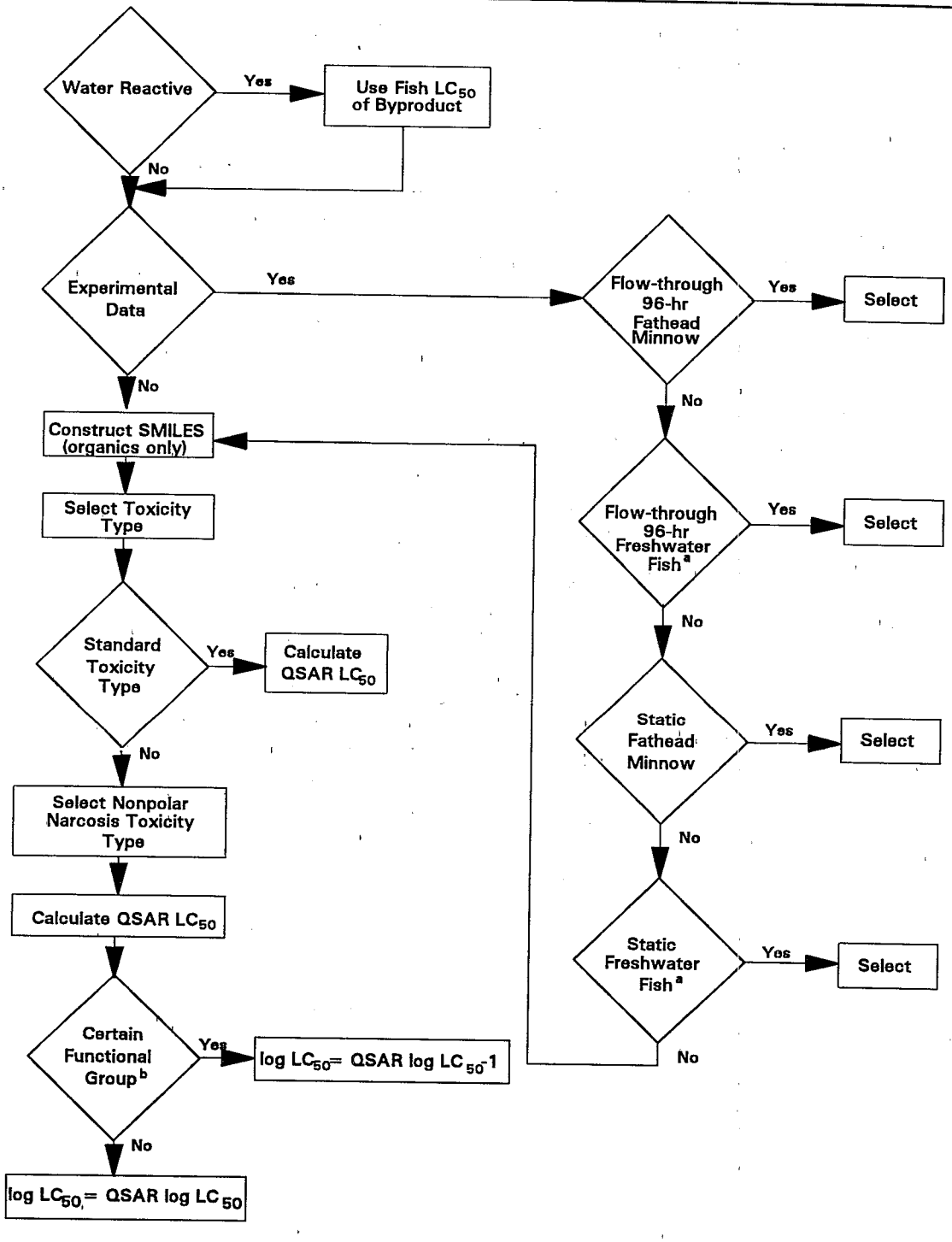
A.2.2 Acute Aquatic Effects

Definitions/Test Methods:

LC_{50}: The concentration of a chemical, in water, that causes death in 50 percent of the fish tested. Acute effects on fish are measured as mortality to *Pimephales promelas* (fathead minnow) in 1) a flow-through 96-hr test and evaluated as log LC_{50} (in mg/l). If data from this test are unavailable, then data is selected from 2) a flow-through 96-hr LC_{50} data for another fresh water fish, or 3) a static 96-hour fathead minnow test or 4) a static 96-hour test for another freshwater fish. In two cases, 48-hour test data were used when 96-hour data were unavailable.

Data Selection

Figure A-6 presents the hierarchy for aquatic LC_{50} data selection. Some functional groups, such as acid chlorides, isocyanates, epoxides, etc., react with water in less than one day. Experimental measurement of the aquatic LC_{50} will, of course, be based on the LC_{50} of the byproducts. When experimental data are absent, the aquatic environmental effects (i.e., fish LC_{50} and fish NOEL) of such compounds calculated using a QSAR were, therefore, taken as those of the hydrolysis products rather than the pollutant itself and the appropriate data substituted into the algorithm. Experimental data from 1) *Acute Toxicities of Organic Chemicals to Fathead Minnows, Volumes 1 through 5* (CLSES, 1984, 1985, 1986, 1988, 1990) and 2) HSDB (1993) are preferred for the acute aquatic toxicity data. Additional data sources were used for the inorganic chemicals, because no valid means of estimating acute aquatic toxicity values for inorganics has been identified (Banerjee and Paul, 1993; Davidson, et al., 1987; Ellgaard and Gilmore, 1984; EPS, 1984; Hose, et al., 1989; IPCS, 1986; IPCS, 1990; IPCS, 1991; Smith, et al., 1985; Spehar et al., 1980; EPA, 1980a; EPA, 1980b; EPA, 1980c; EPA, 1980d; EPA, 1980e; EPA, 1984a; EPA, 1984c). Additional data sources were also used for pesticides (Kidd and James, 1991; EPA, 1984b).



[a] excluding trout

[b] includes good electrophiles, good nucleophiles, strong acids, chemicals with an aromatic ring, and certain reactive groups

Figure A-6. Decision Tree for Fish LC50 Data Selection

If experimental data are not available, but can be estimated by way of a structurally similar compound in the same physical state, a QSAR is used to estimate the acute toxicity value (MICROQSAR 2.0). First, the chemical SMILES (Simplified Molecular Input Line Entry System) was constructed to determine the mechanism of toxic action. SMILES is a chemical nomenclature used to describe organic molecules for computer entry. Based on the toxicity type (e.g., nonpolar narcosis, narcosis, polar narcosis, aniline toxicity, ester narcosis, respiratory uncoupling, aldehyde toxicity, acrylate toxicity, and reactive toxicity) the LC_{50} is calculated as a function of the log K_{ow} using QSARs.

There are certain cases where the molecular structure of a pollutant does not suggest a specific toxic mechanism, so a default nonpolar narcosis was used. For certain functional groups, it is known that their reactivity increases the toxicity beyond what a QSAR based on K_{ow} would predict. These groups include good alkylating agents (electrophiles), good nucleophiles or bases, strong acids and certain reactive groups. For such chemicals, the toxicity was increased over that predicted by default nonpolar narcosis by -1 log unit.

Calculation of Hazard Values

Figure A-7 is a decision tree of the logic used to calculate the fish LC_{50} hazard value. Hazard value scores for the acute aquatic toxicological endpoint were based on the $\log_{10}$ of the LC_{50} values, which were assigned a score between 0 and 5 using a continuous, linear function. Numerical cutoff values were based on commonly accepted cutoffs (Behret, 1989; Foran and Glenn, 1993; Konemann and Visser, 1988; Michigan CMR, 1987). Chemicals with a log K_{ow} greater than 6 were assigned a hazard value of 0.

A.2.3 Fish Chronic Toxicity

Definitions/Test Methods:

No Observable Effect Level (NOEL): The highest dosage administered that does not produce toxic effects (Casarett and Doull, 1986).

Data Selection

Figure A-8 is a decision tree which shows the method for calculating fish NOEL data. Experimental data are generally lacking for the fish NOEL endpoint and were not used in the screening tier. The literature data on fathead minnow acute toxicity provided, in addition to 96-hr LC_{50} data, 96-hr median effect concentration (EC_{50}) data (CLSES, 1984-1990). The EC_{50} values were defined as the concentration causing 50 percent of the fish to show an adverse effect. A comparison of the reported LC_{50} and EC_{50} led to the formulation of the general rules shown in Figure A-8 for estimating the NOEL of organic chemicals from the fish LC_{50} or the log K_{ow}.

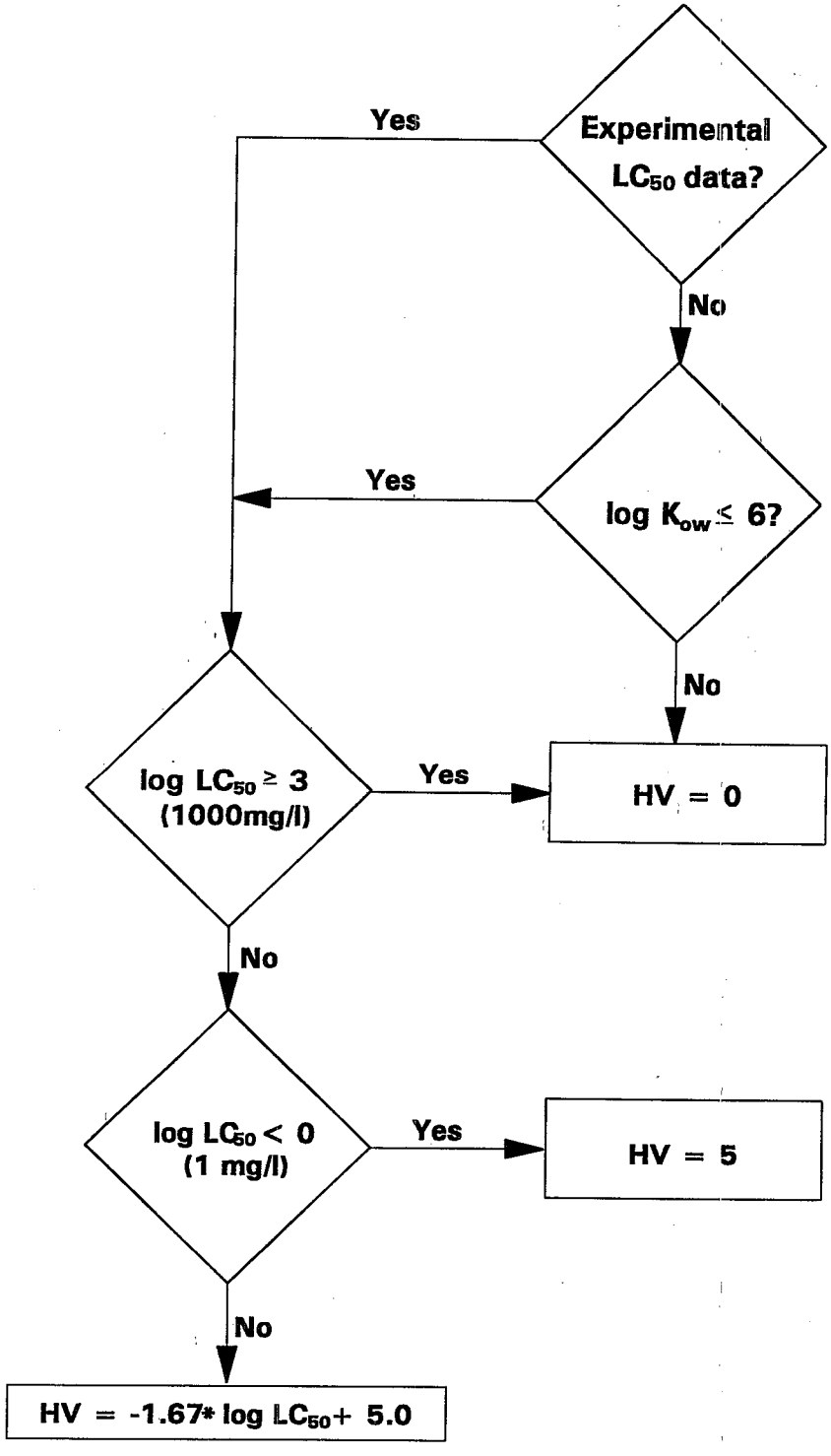


Figure A-7. Decision Tree for Aquatic LC_{50} Hazard Value

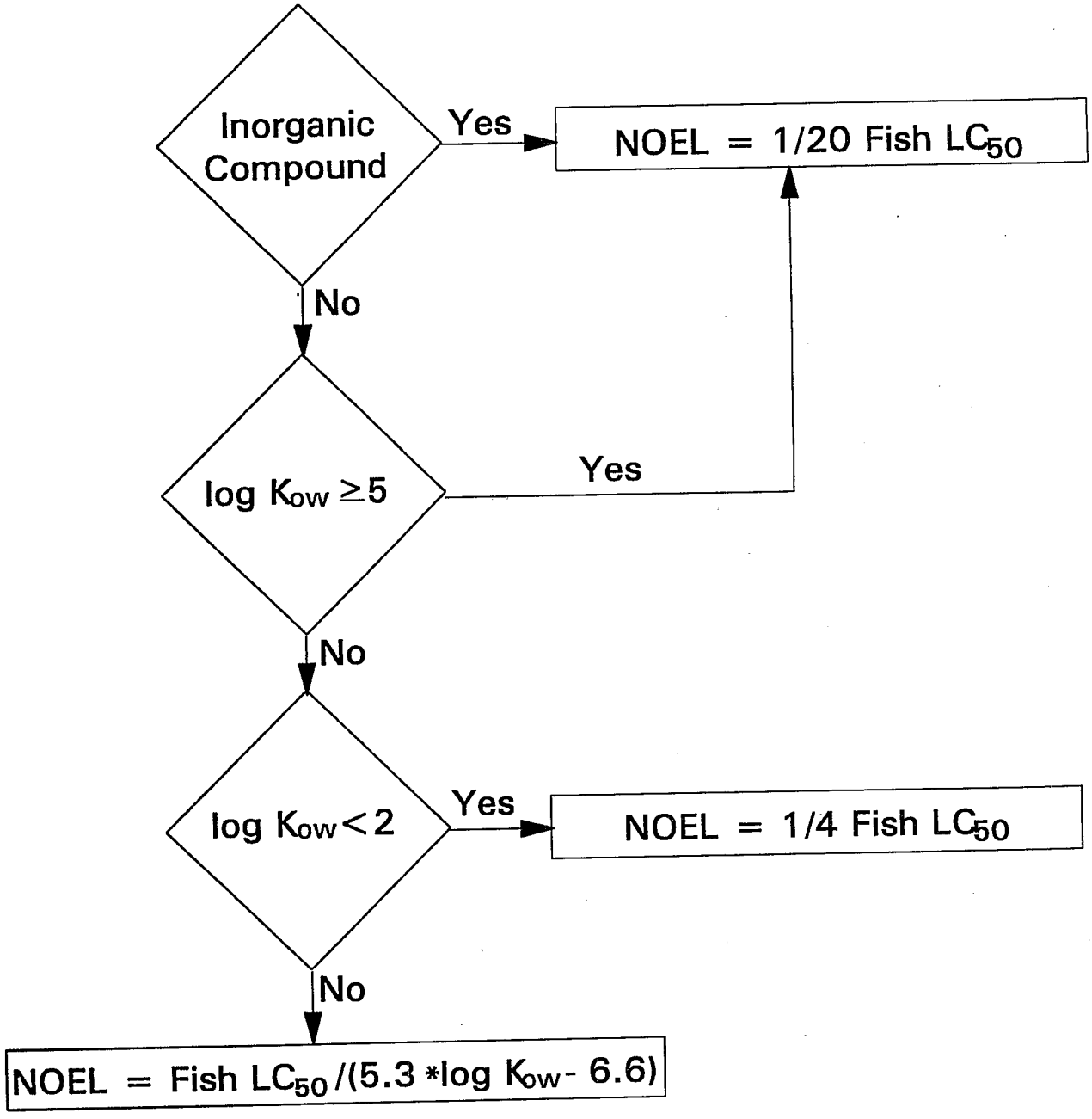


Figure A-8. Decision Tree for Calculating Fish NOEL

The NOEL of the inorganic chemicals is based entirely on the fish LC_{50} since inorganics are poorly fat soluble and their fish toxicity does not correlate to log K_{ow}. Both the fish LC_{50} and log K_{ow} are used to estimate the NOEL of organics. Organic chemicals with a relatively high log K_{ow} (e.g., greater than or equal to 5) are generally more toxic to fish and assigned a lower NOEL compared to organic chemicals with a relatively low log K_{ow} (e.g., less than or equal to 2). The NOEL for the remaining organic chemicals is calculated using a continuous, linear function.

Calculation of Hazard Values

Figure A-9 is a decision tree which shows the method used to calculate the fish NOEL hazard values. Hazard value scores for the subacute aquatic toxicological endpoint were based on the $\log_{10}$ of the NOEL values, which were assigned a score between 0 and 5 using a continuous, linear function. Numerical cutoff values were set one order of magnitude lower than the cutoffs for the fish LC_{50} hazard values.

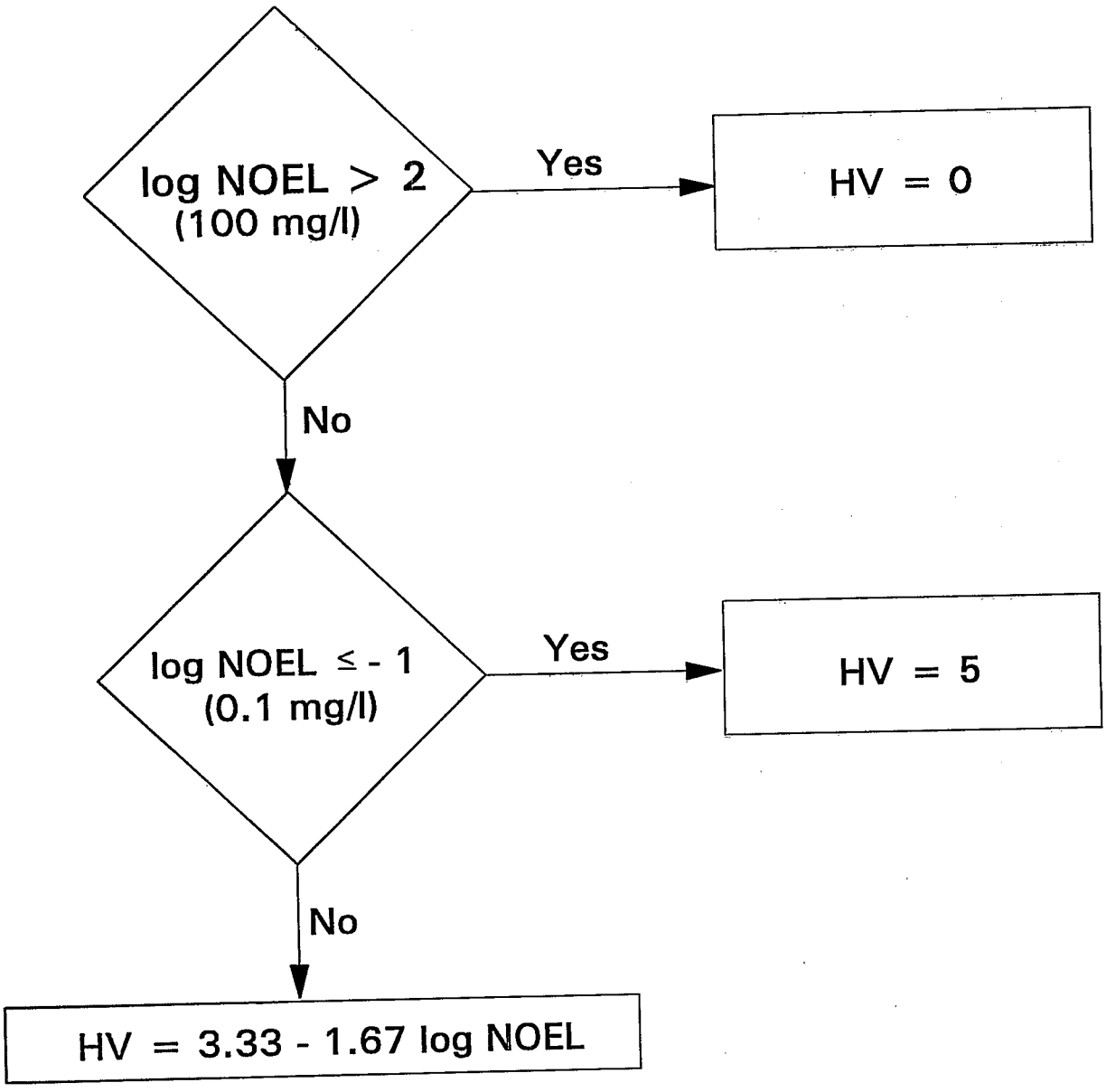


Figure A-9. Decision Tree for NOEL Hazard Value

A.3 EXPOSURE PARAMETERS

A.3.1 Persistence

Definitions/Test Methods:

BOD half-life: The BOD half-life is the time (in days) required for a chemical to biodegrade such that its BOD in water is decreased to half of the original amount.

Hydrolysis half-life: The hydrolysis half-life is the time (in days) required for the amount of a substance to decrease to one-half of the original amount through hydrolysis reaction in water at pH 7.

Data Selection

The BOD half-life of each organic chemical was determined with the computer assisted version (MICROQSAR 2.0) of the structural feature approach developed by Neimi, et al. (1987). This was based on selected literature for 287 chemicals.

Hydrolysis half-life data for the organics, ammonia, chlorine dioxide and hydrochloric acid were determined with the computer assisted version (MICROQSAR version 2.0) of the Hammett and Taft substituent constant methods described by Harris (1981).

Metal compounds and certain other inorganic chemicals in highly oxidized states (e.g., molybdenum trioxide, thorium dioxide, sulfuric acid, nitric acid, and ammonium salts) were assumed to have infinite BOD and hydrolysis half-lives. Zinc and aluminum dusts were assumed to have half-lives of 500 days based on the judgment that they would degrade (oxidize) eventually, although slowly.

Calculation of Hazard Values

Figure A-10 is a decision tree which shows the method used to calculate the BOD half-life hazard values. Figure A-11 is a decision tree which shows the method used to calculate the hydrolysis half-life hazard values. It was decided to use the same scoring criteria for both BOD and hydrolysis half-lives. The criteria were based on the distribution of the half-life data and on the range of values assigned for environmental degradation in other chemical ranking systems in the literature. A maximum hazard value of 2.5 is assigned to BOD or hydrolysis half-lives greater than 500 days and the minimum hazard value of 1.0 is assigned for half-lives less than 4 days. Between 4 and 500 days, the hazard value is calculated between 1 and 2.5 based on a linear scale.

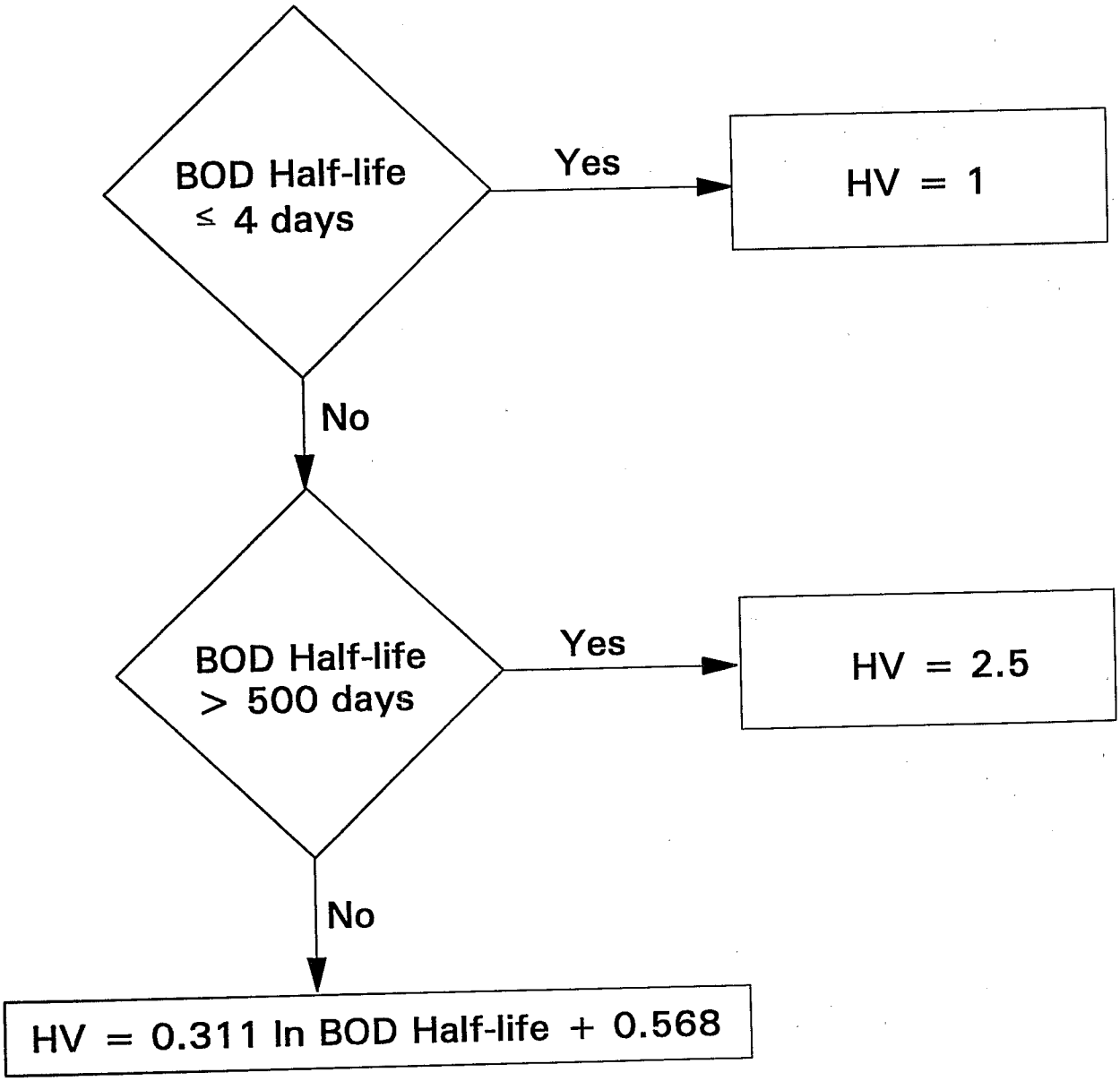


Figure A-10. Decision Tree for BOD Half-Life Hazard Value

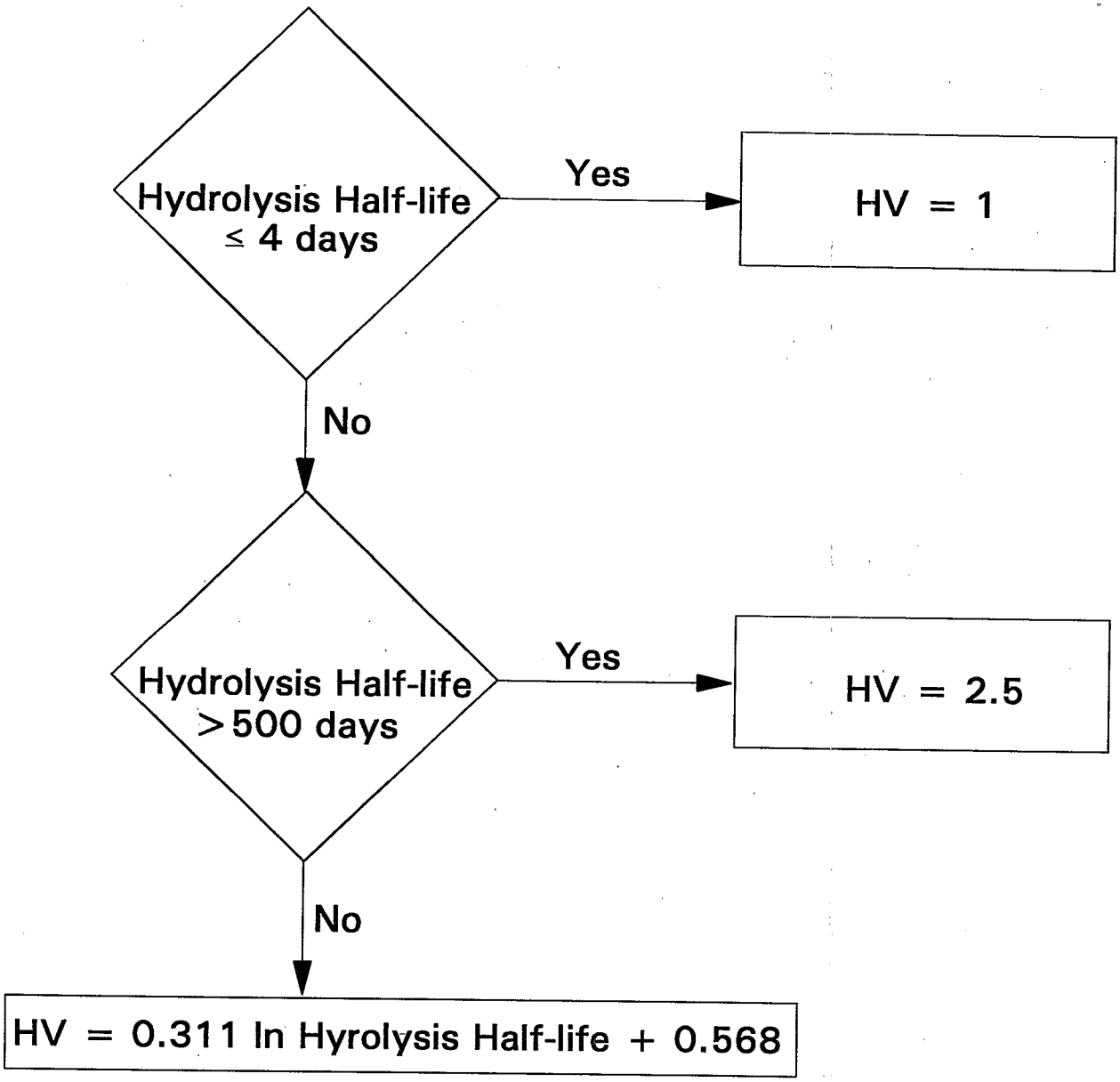


Figure A-11. Decision Tree for Hydrolysis Half-Life Hazard Value

A.3.2 Bioaccumulation

Definitions/Test Methods:

Aquatic Bioconcentration factor (BCF): The ratio of the concentration of a chemical in fish to its concentration in water at steady-state conditions. This factor is a measure of the chemical's ability to bioaccumulate and is typically reported in log units.

Data Selection

The experimental BCF for aquatic organisms can vary by several orders of magnitude depending on specific test parameters and intra- and inter-species differences (size, age, etc.). Therefore, log BCF of each organic chemical was determined using the QSAR equation developed by Bintein et al., (1993) which considers these differences: log BCF = 0.910 log K_{ow} - 1.975 log (6.8 10^{-7} K_{ow} + 1) - 0.786. Experimental log BCF data tabulated by EPA was used when available for inorganic chemicals (EPA, 1979). Numerical values for barium and cobalt compounds were based on ranges of BCF values from HSDB. Otherwise, the log BCF endpoint was flagged as missing data and no hazard value was assigned.

Calculation of Hazard Values

Figure A-12 presents the method used to calculate the log BCF hazard values. The BCF value increases with increasing K_{ow} until the log K_{ow} reaches a value of approximately 6. Beyond a log K_{ow} of 6, the BCF drops off. Using this model, the maximum possible log BCF is approximately 4.5. Based on this range of BCF values, a maximum hazard value of 2.5 is assigned for log BCF $\geq$ 4 and the minimum hazard value of 1.0 is assigned for log BCF $\leq$ 1. Between log BCF of 1 and 4, the hazard value is calculated between 1.0 and 2.5 based on a linear scale.

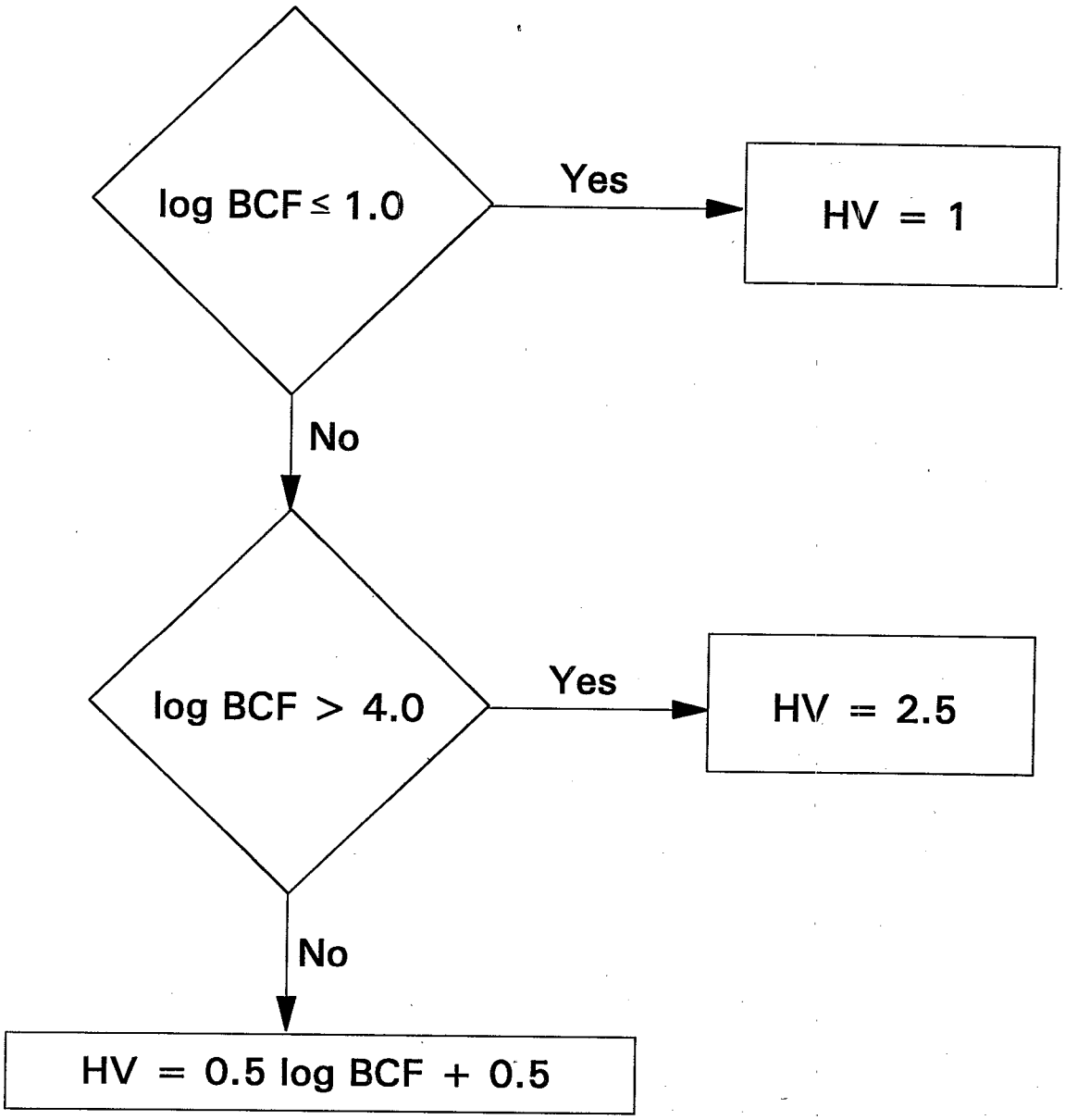


Figure A-12. Decision Tree for BCF Hazard Value

A.4 WEIGHTING BY RELEASES

The final hazard value considers both the intrinsic properties of each chemical and the likelihood of exposure. The hazard values assigned to the toxicological endpoints are multiplied by a release weighting factor (RWF) based on the appropriate type of TRI releases or transfers to air or water.

Definitions

Release weighting factor (RWF): A multiplicative factor used to weight toxicity hazard values for each chemical according to the amount of its annual releases or transfers to air and water, where

$$RWF = \ln releases - 10$$

Data Selection

Data for the releases and transfers for the industrial chemicals were obtained from the 1989 TRI. Releases for pesticides, which are intentionally released, were obtained from annual usage information for 1987 (EPA, 1988b), 1990 and 1991 (Aspelin et al., 1992).

All releases were classified as either air or water releases. It is assumed that stack and fugitive releases went to air, and that land, injection, water, and POTW releases went to water. Off-site transfers to an incineration or recycling facility were assumed destroyed or not released to the environment. All other off-site transfers were assumed released to water.

A method was developed for scoring the releases on a smooth scale from 1 to 10 on a logarithmic basis. Using the natural log (ln) gives the data a normal distribution. The natural log, rather than the base-10 log, was used to attain a range of 10 integers over the range of release amounts. Total releases for the chemicals scored ranged from 860 lbs. to 545,989,541 lbs. The equation for calculating the RWF results in the assignment of a multiplier of approximately 10 for the highest release and a 1 for anything that is 59,874 lbs or less. By subtracting 10 from the natural log of the releases, a cutoff of 60,000 lbs. is set, below which the weighting factor is always equal to one.

Calculation of Hazard Values

Although it is understood that releases to one medium can result in exposure by multiple routes, for the purpose of simplicity in this screening tier, it was assumed that air releases would result in inhalatory exposure and that water releases would result in oral exposure as well as exposure to aquatic organisms. Fugacity modelling in the next tier is expected to provide more realistic assumptions. The RWF was applied in the following manner:

- The weighting factor for air releases (RWF_{air}) was applied to the hazard value assigned for the inhalation rodent LC_{50}.
- The weighting factor for water releases (RWF_{water}) was applied to the oral rodent LD_{50}, fish LC_{50}, and fish NOEL.

- The weighting factor for the total air and water releases (RWF_{total}) was applied to the chronic toxicological endpoints for carcinogenicity and "other specific effects."

Therefore, the final weighted hazard values (wHV) for the human health effects and the environmental effects were obtained as follows:

$$\text{Weighted Human Health Effects} = (HV_{\text{oral LD50}})(RWF_{water}) + (HV_{\text{inhal LC50}})(RWF_{air}) + (HV_{carcin} + HV_{other})(RWF_{total})$$

$$\text{Weighted Environmental Effects} = (HV_{\text{oral LD50}} + HV_{\text{fish LC50}} + HV_{\text{fishNOEL}})(RWF_{water})$$

The Exposure Factor remains unchanged where:

$$\text{Exposure Factor} = HV_{BOD} + HV_{hydrolysis} + HV_{BCF}$$

The final total wHV for each chemical is obtained as follows:

$$wHV = (\text{weighted Human Health Effects} + \text{weighted Env. Effects}) * \text{Exposure Factor}$$

These numbers provide the basis for the ranking of all scored chemicals.

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APPENDIX B
TRI CHEMICALS AND HIGH-VOLUME PESTICIDES

CHEMICALS SELECTED FROM 1989 TRI BASED ON 99% OF TOTAL RELEASES

Selected Chemicals	Original list of Chemicals
X	1,1,1-trichloroethane
	1,1,2,2-tetrachloroethane
X	1,1,2-trichloroethane
	1,1-dimethyl hydrazine
X	1,2,4-trichlorobenzene
X	1,2,4-trimethylbenzene (pseudocumeme)
	1,2-butylene oxide
	1,2-dibromoethane
X	1,2-dichlorobenzene
X	1,2-dichloroethane
	1,2-dichloroethylene
X	1,2-dichloropropane
X	1,3-butadiene
	1,3-dichlorobenzene
	1,3-dichloropropylene
X	1,4-dichlorobenzene
X	1,4-dioxane
	2,4,5-trichlorophenol
	2,4,6-trichlorophenol
X	2,4-D
	2,4-diaminoanisole
	2,4-diaminoanisole sulfate
	2,4-diaminotoluene
	2,4-dichlorophenol
	2,4-dimethylphenol
X	2,4-dinitrophenol
X	2,4-dinitrotoluene
	2,5-dichloro-3-aminobenzoic acid
	2,6-dinitrotoluene
	2,6-xylidine
X	2-ethoxyethanol
X	2-methoxyethanol
	2-nitrophenol
X	2-nitropropane
	2-phenylphenol
	3,3'-dichlorobenzidine
	3,3'-dimethoxybenzidine
	3,3'-dimethylbenzidine
	4,4'-diaminodiphenyl ether
X	4,4'-isopropylidenediphenol
	4,4'-methylenebis(2-Cl-aniline)(mboca)
X	4,4'-methylenedianiline
	4,6-dinitro-o-cresol
	4-aminoazobenzene
	4-aminobiphenyl
X	4-nitrophenol
	5-nitro-o-anisidine
X	Acetaldehyde
	Acetamide
X	Acetone
X	Acetonitrile
	Acrolein
X	Acrylamide
X	Acrylic acid
X	Acrylonitrile

Selected Chemicals	Original list of Chemicals
X	Allyl chloride
	Alpha-naphthylamine
X	Aluminum (fume or dust)
X	Ammonia
X	Ammonium nitrate (solution)
X	Ammonium sulfate (solution)
X	Aniline
X	Anthracene
	Antimony
X	Antimony compounds
	Arsenic
X	Arsenic compounds
X	Asbestos (friable)
	Barium
X	Barium compounds
	Benzal chloride
	Benzamide
X	Benzene
	Benzoic trichloride
X	Benzoyl chloride
	Benzoyl peroxide
	Benzyl chloride
	Beryllium
	Beryllium compounds
X	Biphenyl
	Bis(2-chloro-1-methylethyl) ether
	Bis(2-chloroethyl) ether
X	Bis(2-ethylhexyl) adipate
	Bis(chloromethyl) ether
	Bromoform
X	Bromomethane
X	Butyl acrylate
X	Butyl benzyl phthalate
X	Butyraldehyde
	C.i. basic green 4 (Malachite Green Oxal
	C.i. basic red 1 (Rhodamin 6G)
	C.i. direct black 38
	C.i. disperse yellow 3
	C.i. solvent yellow 14 (Sudan I)
	C.i.food red 15
	Cadmium
X	Cadmium compounds
	Calcium cyanamide
	Captan
	Carbaryl
X	Carbon disulfide
X	Carbon tetrachloride
X	Carbonyl sulfide
X	Catechol
	Chlordane
X	Chlorine
X	Chlorine dioxide
	Chloroacetic acid
X	Chlorobenzene
X	Chloroethane

CHEMICALS SELECTED FROM 1989 TRI BASED ON 99% OF TOTAL RELEASES

Selected Chemicals	Original list of Chemicals
X	Chloroform
X	Chloromethane
	Chloromethyl methyl ether
X	Chlorophenols
X	Chloroprene
X	Chlorothalonil
	Chromium
X	Chromium compounds
	Cobalt
X	Cobalt compounds
	Copper
X	Copper compounds
X	Cresol (mixed isomers)
X	Cumene
X	Cumene hydroperoxide.
	Cupferron
	Cyanide compounds
X	Cyclohexane
X	Decabromodiphenyl oxide
X	Di(2-ethylhexyl) phthalate
X	Diaminotoluene (mixed isomers) 2,4
	Dibenzofuran
X	Dibutyl phthalate
X	Dichlorobenzene (mixed isomers)
X	Dichloromethane
	Dichlorvos
	Dicofol
X	Diethanolamine
X	Diethyl phthalate
	Diethyl sulfate
X	Dimethyl phthalate
	Dimethyl sulfate
X	Epichlorohydrin
	Ethoxylated C10-C16 Alcohols
	Ethyl acrylate
	Ethyl chloroformate
X	Ethylbenzene
X	Ethylene
X	Ethylene glycol
X	Ethylene oxide
	Ethylene thiourea
	Fluometuron
X	Formaldehyde
X	Freon 113
X	Glycol ethers (use tri)
	Heptachlor
X	Hexachloro-1,3-butadiene
X	Hexachlorobenzene
	Hexachlorocyclopentadiene
X	Hexachloroethane
	Hydrazine
	Hydrazine sulfate
X	Hydrochloric acid
X	Hydrogen cyanide
X	Hydrogen fluoride

Selected Chemicals	Original list of Chemicals
X	Hydroquinone
X	Isobutyraldehyde
X	Isopropyl alcohol (manufacturing,
	Lead
X	Lead compounds
	Lindane
	M-cresol
X	M-xylene
X	Maleic anhydride
	Maneb
	Manganese
X	Manganese compounds
	Mercury
	Mercury compounds
X	Methanol
	Methoxychlor
	Methyl acrylate
X	Methyl ethyl ketone
	Methyl hydrazine
	Methyl iodide
X	Methyl isobutyl ketone
	Methyl isocyanate
X	Methyl methacrylate
X	Methyl tert-butyl ether
	Methylene bromide
X	Methylenebis(phenylisocyanate)
	Michler's ketone
X	Molybdenum trioxide
X	N,N-dimethylaniline
X	N-butyl alcohol
X	N-dioctyl phthalate
	N-nitrosodimethylamine
X	N-nitrosodiphenylamine
X	Naphthalene
	Nickel
X	Nickel compounds
X	Nitric acid
	Nitrilotriacetic acid
X	Nitrobenzene
	Nitroglycerin
	O-anisidine
	O-cresol
	O-toluidine
X	O-xylene
	P-anisidine
	P-cresidine
X	P-cresol
	P-nitrosodiphenylamine
	P-phenylenediamine
X	P-xylene
	Parathion
	Pentachlorophenol
	Peracetic acid
X	Phenol
	Phosgene

CHEMICALS SELECTED FROM 1989 TRI BASED ON 99% OF TOTAL RELEASES

Selected Chemicals	Original list of Chemicals
X	Phosphoric acid
X	Phosphorus (yellow or white)
X	Phthalic anhydride
X	Picric acid
X	Polychlorinated biphenyls
X	Propionaldehyde
	Propoxur
X	Propylene
X	Propylene oxide
	Propyleneimine
X	Pyridine
	Quinoline
	Quinone
	Quintozene
	Saccharin (manufacturing only)
	Safrole
X	Sec-butyl alcohol
	Selenium
	Selenium compounds
	Silver
	Silver compounds
X	Styrene
	Styrene oxide
X	Sulfuric acid
X	Terephthalic acid
X	Tert-butyl alcohol
X	Tetrachloroethylene
	Tetrachlorvinphos
	Thallium
	Thallium compounds
	Thiourea
X	Thorium dioxide
X	Titanium tetrachloride
X	Toluene
X	Toluene-2,4-diisocyanate
	Toluene-2,6-diisocyanate
	Trichlorfon
X	Trichloroethylene
	Urethane
	Vanadium (fume or dust)
X	Vinyl acetate
	Vinyl bromide
X	Vinyl chloride
X	Vinylidene chloride
X	Xylene (mixed isomers)
X	Zinc (fume or dust)
X	Zinc compounds
	Zineb
	other mixtures or trade names

HIGH VOLUME PESTICIDES SELECTED
Alachlor
Atrazine
Butylate
Captan
Carbaryl
Chlorpyrifos
Cyanazine
1,3-Dichloropropene
EPTC
Glyphosate
Malathion
Maneb
Metam-sodium
Methyl parathion
Metolachlor
Metribuzin
Terbufos
Trifluralin

APPENDIX C
RANKING RESULTS: HORIZONTAL TABLES

HORIZONTAL TABLE: ALGORITHM 10/7/93, DEFAULT HV TO 0 FOR MISSING DATA

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
sec-butyl alcohol	0.6	6480	0	8000	0.2	0	0	3670	0	918	0	9	1.25	1000	2.5	-0.2	1	0	0.19	0	4.75	0.9	
Glyphosate	-3.3	4873	0	-99	0	0	0	600	0.4	150	0	9	1.25	1000	2.5	-3.7	1	0	0.02	0.39	4.75	1.9	I
Methyl tert-butyl ether	0.9	4000	0.2	23568	0	0	0	786	0.2	197	0	508	2.5	1000	2.5	0	1	0	0.16	0.34	6	3	
tert-butyl alcohol	0.4	3500	0.3	8000	0.2	0	0	1954	0	488	0	508	2.5	1000	2.5	-0.5	1	0	0.45	0.26	6	4.3	
Ammonium sulfate (solution)	0	3000	0.4	-99	0	0	0	4000	0	200	0	9999	2.5	9999	2.5	-2	1	0	0.37	0.37	6	4.4	KI
Methanol	-0.6	5628	0	64000	0	0	1	29400	0	7350	0	9	1.25	1000	2.5	-1.4	1	0	1	0	4.75	4.8	
Carbonyl sulfide	0.1	0	0	10000	0	0	1	2685	0	671	0	9999	2.5	1000	2.5	-0.7	1	0	1	0	6	6	
Acetone	-0.2	3000	0.4	42000	0	0	1	7200	0	1800	0	7	1.15	1000	2.5	-1	1	0	1.37	0.37	4.65	8.1	
Acetonitrile	-0.3	3800	0.2	15000	0	0	3	1640	0	410	0	5	1.07	1	1	-1.1	1	0	3.2	0.2	3.07	10.4	
Freon 113	1.7	43000	0	10000	0	0	1	290	0.9	73	0.2	503	2.5	30	1.63	0.7	1	0	1	1.13	5.13	10.9	
Ammonium nitrate (solution)	0	4500	0.1	-99	0	0	1	800	0.2	40	0.7	9999	2.5	9999	2.5	-2	1	0	1.08	0.9	6	11.9	KI
Thorium dioxide	0	1140	1.1	-99	0	0	0	-99	0	-99	0	9999	2.5	9999	2.5	-99	1	0	1.07	1.07	6	12.8	KIFNc
Ethylene glycol	-1.9	6610	0	1000	2	0	1	227634	0	56909	0	9	1.25	1000	2.5	-2.5	1	0	3	0	4.75	14.3	
Aluminum (fume or dust)	0	9999	0	500	2.6	0	0	-99	0	-99	0	500	2.5	9999	2.5	-99	1	0	2.6	0	6	15.6	KFNc
Antimony cmpds	0	20000	0	-99	0	0	2	833	0.1	42	0.6	9999	2.5	9999	2.5	1.6	1.3	0	2	0.77	6.3	17.4	KI
Metribuzin	1.7	7500	0	-99	0	0	0	80	1.8	20	1.2	508	2.5	1000	2.5	0.8	1	0	0	2.99	6	18	I
n-butyl alcohol	0.9	790	1.3	8000	0.2	0	1	1860	0	465	0	9	1.25	1000	2.5	0	1	0	2.53	1.34	4.75	18.4	
Methyl isobutyl ketone	1.2	2080	0.6	5672	0.5	0	2	505	0.5	126	0	7	1.15	1000	2.5	0.3	1	0	3.13	1.13	4.65	19.8	
1,2-Dichloropropane	2.3	3000	0.4	5554	0.5	0	0	127	1.5	23	1.1	503	2.5	30	1.63	1.3	1.14	0	0.88	2.92	5.27	20	
Methyl methacrylate	1.4	8000	0	7500	0.2	0	3	259	1	65	0.3	9	1.25	1000	2.5	0.5	1	0	3.25	1.29	4.75	21.6	
Glycol ethers	0.8	1200	1	450	2.7	0	0	1490	0	373	0	9	1.25	1000	2.5	0	1	0	3.73	1.03	4.75	22.6	
Methyl ethyl ketone	0.3	2737	0.4	6766	0.3	0	4	3220	0	805	0	7	1.15	1000	2.5	-0.5	1	0	4.78	0.44	4.65	24.2	
Butyraldehyde	0.9	2490	0.5	7547	0.2	0	0	32	2.5	8	1.8	7	1.15	1000	2.5	0	1	1	0.75	4.82	4.65	25.9	
Diethanolamine	-1.4	710	1.4	484	2.6	0	0	4710	0	1178	0	9	1.25	1000	2.5	-2.1	1	0	4.04	1.41	4.75	25.9	
1,4-Dioxane	-0.3	3150	0.3	6368	0.4	3.5	0	10352	0	2588	0	520	2.5	1000	2.5	-1	1	0	4.23	0.33	6	27.4	
Phthalic anhydride	1.3	2000	0.7	1000	2	0	2	364	0.7	91	0.1	550	2.5	1000	1	0.4	1	2	4.66	1.46	4.5	27.6	
2-ethoxyethanol	-0.5	1400	0.9	3185	1	0	3	16305	0	4076	0	9	1.25	1000	2.5	-1.3	1	0	4.92	0.92	4.75	27.7	
Chloromethane	0.9	1800	0.7	3063	1	1.5	3	550	0.4	138	0	6	1.13	30	1.63	0	1	0	6.27	1.17	3.75	27.9	
Dimethyl phthalate	1.3	2400	0.5	500	2.6	0	0	121	1.5	30	0.9	9	1.25	400	2.43	0.4	1	0	3.13	2.93	4.68	28.4	
Isobutyraldehyde	0.6	2810	0.4	6681	0.4	0	1	41	2.3	10	1.6	7	1.15	1000	2.5	-0.2	1	1	1.77	4.37	4.65	28.6	
Vinyl acetate	0.7	1613	0.8	3680	0.9	0	1	100	1.7	25	1	9	1.25	1000	2.5	-0.1	1	0	2.69	3.49	4.75	29.4	
Zinc (fume or dust)	0	9999	0	1000	2	0	3	-99	0	-99	0	500	2.5	9999	2.5	-2	1	0	5	0	6	30	KFN
Maleic anhydride	0.1	465	1.7	1000	2	3	1	2963	0	741	0	8	1.2	1000	1	-0.7	1	2	7.72	1.72	3.2	30.2	
2-methoxyethanol	-0.8	950	1.2	2590	1.2	0	3	22655	0	5664	0	9	1.25	1000	2.5	-1.5	1	0	5.38	1.2	4.75	31.3	
Ethylene	1.1	9999	0	950000	0	0	1	14	3.1	3	2.4	10	1.28	1000	2.5	0.2	1	0	1	5.55	4.78	31.4	
Terephthalic acid	1.6	18800	0	-99	0	0	1	29	2.6	7	1.9	550	2.5	1000	2.5	0.7	1	0	1	4.45	6	32.7	I
Propylene	1.8	9999	0	10500	0	0	0	5	3.8	1	3.2	10	1.28	1000	2.5	0.8	1	0	0	6.97	4.78	33.4	
Hydroquinone	0.6	320	2	-99	0	0	1	141	1.4	35	0.8	9	1.25	1000	2.5	-0.2	1	0	2.99	4.17	4.75	34	I
Pyridine	0.6	1580	0.8	1000	2	0	1	100	1.7	25	1	9	1.23	1000	2.5	-0.2	1	0	3.83	3.51	4.73	34.7	
Nitrobenzene	1.9	640	1.5	-99	0	0	2	119	1.5	30	0.9	9	1.23	1000	2.5	0.9	1	0	3.49	3.91	4.73	35	I
Diethyl phthalate	2.5	9000	0	537	2.5	0	0	32	2.5	5	2.2	9	1.25	400	2.43	1.5	1.23	0	2.54	4.68	4.91	35.5	
Isopropyl alcohol	0.3	3600	0.2	32000	0	5	2	8623	0	2156	0	9	1.25	1000	2.5	-0.5	1	0	7.24	0.24	4.75	35.5	
Toluene	2.7	5050	0	6675	0.4	0	2	34	2.4	4	2.3	10	1.27	1000	2.5	1.7	1.33	0	2.35	4.7	5.1	36	
Asbestos (friable)	0	9999	0	9999	0	5	1	-99	0	-99	0	9999	2.5	9999	2.5	1	1	0	6	0	6	36	KFN
Dichloromethane	1.3	1600	0.8	17400	0	3.5	1	330	0.8	83	0.1	508	2.5	30	1.63	0.4	1	0	5.32	1.77	5.13	36.4	
Metolachlor	3.5	2780	0.4	-99	0	0	0	15	3	1	3.2	503	2.5	2	1	2.4	1.68	2	0.43	6.62	5.18	36.5	I
Benzoyl chloride	2.2	2460	0.5	163	3.6	0	2	35	2.4	7	1.9	9	1.25	1000	1	1.2	1.12	2	6.09	4.89	3.37	37	
Chloroethane	1.4	7500	0	29	5	0	0	16	3	4	2.3	6	1.13	30	1.63	0.5	1	0	5	5.29	3.75	38.6	
Butylate	3.7	4659	0.1	-99	0	0	0	7	3.6	0.54	3.8	518	2.5	1000	1	2.5	1.77	2	0.05	7.43	5.27	39.4	I
Carbon disulfide	0.8	2780	0.4	1604	1.6	0	4	694	0.3	174	0	9999	2.5	1000	2.5	0	1	0	6.01	0.69	6	40.2	

HORIZONTAL TABLE: ALGORITHM 10/7/93, DEFAULT HV TO 0 FOR MISSING DATA

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
Maneb	0	4400	0.1	-99	0	0	4	2	4.6	0.09	5	-99	1	-99	1	-99	1	0	4.09	9.67	3	41.3	Klbhc
Allyl chloride	-0.2	425	1.8	926	2.1	1.5	3	72	1.9	18	1.2	6	1.13	2	1	-1	1	0	8.35	4.92	3.13	41.5	
Butyl benzyl phthalate	4.8	2330	0.6	-99	0	0	1	43	2.3	2	2.7	8	1.2	400	2.43	3.5	2.26	0	1.55	5.56	5.89	41.9	I
Butyl acrylate	2.4	3730	0.2	2730	1.1	0	0	2	4.6	0.31	4.2	9	1.25	50	1.78	1.4	1.18	0	1.34	8.94	4.22	43.3	
Acrylic acid	0.4	193	2.4	1200	1.8	0	1	186	1.2	47	0.6	8	1.2	1000	2.5	-0.5	1	0	5.2	4.13	4.7	43.8	
Zinc compounds	0	7950	0	-99	0	0	0	17	2.9	0.86	3.4	9999	2.5	9999	2.5	3	2	0	0	6.39	7	44.7	Kl
EPTC (ethyl dipropylthiocarbamate)	3.2	916	1.2	4062	0.8	0	0	27	2.6	3	2.6	9	1.25	1000	2.5	2.1	1.56	1	2.01	6.48	5.31	45.1	
1,1,1-Trichloroethane	2.5	11240	0	2000	1.4	0	3	48	2.2	7	1.9	503	2.5	30	1.63	1.5	1.24	0	4.4	4.11	5.37	45.6	
m-Xylene	3.2	5000	0	4550	0.7	0	2	16	3	2	3	10	1.27	1000	2.5	2.1	1.56	0	2.68	6.01	5.33	46.4	
Propylene oxide	0	690	1.4	1740	1.5	4	5	306	0.9	77	0.2	9	1.25	1000	1	-0.8	1	2	11.95	2.48	3.25	46.9	
Carbaryl	2.4	500	1.7	25000	0	0	4	8	3.5	1	3.2	8	1.22	1000	1	1.4	1.18	2	5.67	8.35	3.4	47.6	
o-Xylene	2.8	5000	0	4550	0.7	0	3	16	3	2	2.8	10	1.27	1000	2.5	1.7	1.37	0	3.68	5.8	5.14	48.7	
Propionaldehyde	0.3	1200	1	4581	0.7	3	1	44	2.3	11	1.6	7	1.15	1000	2.5	-0.5	1	1	5.71	4.9	4.65	49.4	
Catechol	0.9	260	2.1	-99	0	0	0	9	3.4	2	2.7	9	1.25	1000	2.5	0	1	0	2.14	8.26	4.75	49.4	I
Alachlor	3.1	1065	1.1	-99	0	0	0	5	3.8	0.51	3.8	503	2.5	2	1	2	1.51	2	1.12	8.77	5.01	49.6	f
Acetaldehyde	-0.2	1930	0.7	1500	1.6	3.5	0	34	2.4	9	1.8	7	1.15	1000	2.5	-1	1	1	5.84	4.92	4.65	50	f
Xylene (mixed isomers)	3	4300	0.1	6350	0.4	0	3	13	3.1	1	3.1	10	1.27	1000	2.5	1.9	1.47	0	3.5	6.3	5.24	51.4	
Aniline	0.9	250	2.2	306	3	0	1	108	1.6	27	0.9	9	1.25	1000	2.5	0	1	0	6.2	4.73	4.75	51.9	
Methylenebis(phenylisocyanate)	3.4	2200	0.6	5	5	0	0	66	2	6	2.1	550	2.5	1000	1	2.3	1.64	2	5.59	4.62	5.14	52.6	
1,2,4-Trimethylbenzene	3.4	5000	0	3655	0.9	0	0	8	3.5	0.68	3.6	502	2.5	1000	2.5	2.3	1.65	0	0.87	7.14	6.65	53.3	
Metam Sodium (MeNHCS2Na)	1	285	2.1	888	2.1	0	0	0.39	5	0.1	5	10	1.28	1	1	0.1	1	1	4.18	12.07	3.28	53.4	
Ethylbenzene	3.2	5460	0	5000	0.6	0	3	11	3.3	1	3.3	10	1.27	1000	2.5	2.1	1.54	0	3.6	6.59	5.31	54.1	
Bromomethane	1.2	214	2.3	780	2.2	0	2	11	3.3	3	2.6	6	1.13	30	1.63	0.3	1	0	6.5	8.15	3.75	54.9	
Manganese cmpds	0	615	1.5	-99	0	0	3	150	1.4	8	1.9	9999	2.5	9999	2.5	1	1	0	4.52	4.77	6	55.7	Kl
Molybdenum trioxide	0	125	2.7	-99	0	0	2	370	0.7	19	1.2	9999	2.5	9999	2.5	-99	1	0	4.67	4.61	6	55.7	Klc
Picric acid	2	30	3.7	-99	0	0	0	170	1.3	41	0.6	550	2.5	1000	2.5	1.1	1.03	0	3.7	5.63	6.03	56.3	I
N,N-Dimethylaniline	2.3	1410	0.9	1225	1.8	0	2	65	2	12	1.6	513	2.5	1000	2.5	1.3	1.16	0	4.74	4.45	6.16	56.6	
Cumene hydroperoxide	2.3	382	1.9	200	3.4	1	0	62	2	11	1.6	9	1.23	1000	2.5	1.3	1.14	0	6.26	5.45	4.87	57	
Cyanazine	1.9	261	2.1	230	3.3	0	0	18	2.9	5	2.2	503	2.5	1	1	0.9	1	2	5.41	7.29	4.5	57.2	
Chlorobenzene	2.8	1440	0.9	1100	1.9	0	2	17	3	2	2.8	6	1.13	1000	2.5	1.8	1.4	0	4.82	6.69	5.02	57.8	
Toluene-2,4-diisocyanate	1.8	5800	0	10	5	3.5	1	53	2.1	13	1.5	550	2.5	1000	1	0.8	1	2	9.5	3.6	4.5	58.9	
Atrazine	2.3	1750	0.8	540	2.5	0	0	16	3	3	2.6	503	2.5	1000	2.5	1.3	1.17	0	3.3	6.35	6.17	59.5	
Barium cmpds	0	132	2.6	-99	0	0	2	200	1.2	10	1.7	9999	2.5	9999	2.5	1	1	0	4.63	5.46	6	60.6	Kl
Chlorine dioxide	0	292	2.1	130	3.8	0	2	0.17	5	0.01	5	5	1.07	1	1	-99	1	0	7.83	12.06	3.07	61	Kc
Hydrochloric acid	1.1	900	1.2	277	3.1	0	1	19	2.9	0.95	3.4	10	1.28	1000	2.5	0.5	1	1	5.36	7.48	4.78	61.4	
p-Xylene	3.2	5000	0	4550	0.7	0	2	2	4.5	0.2	4.5	10	1.27	1000	2.5	2.1	1.54	0	2.68	9	5.31	62	
1,4-Dichlorobenzene	3.4	3790	0.2	1100	1.9	3.5	1	34	2.5	3	2.5	6	1.13	1000	2.5	2.3	1.65	0	6.62	5.2	5.27	62.3	
Benzene	2.1	4700	0	17500	0	5	3	19	2.9	4	2.3	10	1.27	1000	2.5	1.2	1.08	0	8.04	5.26	4.84	64.5	
Chloroform	2	908	1.2	5720	0.5	3.5	3	71	1.9	18	1.3	503	2.5	30	1.63	1	1	0	8.22	4.41	5.13	64.8	
Chlorophenols [o]	2.3	261	2.1	100	4	0	0	19	2.9	3	2.4	6	1.13	1000	2.5	1.3	1.15	0	6.14	7.45	4.78	64.9	
4,4'-Isopropylidenediphenol	3.3	2500	0.5	200	3.4	0	0	5	3.9	0.42	4	8	1.2	1000	2.5	2.2	1.62	0	3.9	8.36	5.31	65.1	
Carbon tetrachloride	2.8	2800	0.4	19052	0	3.5	3	41	2.3	5	2.2	503	2.5	30	1.63	1.8	1.39	0	6.92	4.9	5.52	65.3	
p-Cresol	2	207	2.3	50	4.6	0	0	25	2.7	6	2	9	1.23	1000	2.5	1	1	0	6.91	6.98	4.73	65.8	
Acrylonitrile	-0.9	78	3	576	2.5	4	3	10	3.3	3	2.7	5	1.07	1	1	-1.6	1	0	12.49	9	3.07	66	
Phosphorus (yellow or white)	3	3	5	-99	0	0	2	0.02	5	0	5	-99	1	0	1	1	1	0	7	15	3	66	Ib
Cresol (mixed isomers)	2	760	1.4	50	4.6	0	1	13	3.2	3	2.5	9	1.23	1000	2.5	1	1	0	6.97	7.01	4.73	66.2	
Malathion	2.9	570	1.6	6	5	0	0	0.1	5	0.01	5	9	1.25	1000	1	1.8	1.4	2	6.57	11.57	3.66	66.3	
Phosphoric acid	-0.6	1530	0.9	14	5	0	0	70	1.9	4	2.4	9999	2.5	1000	2.5	-0.9	1	1	5.86	5.21	6	66.4	
Di-n-octyl phthalate	5.2	13000	0	-99	0	0	1	0.93	5	0.05	5	9	1.23	400	2.43	3.9	2.44	0	1	10	6.1	67.1	I
Phenol	1.5	530	1.6	46	4.7	0	2	34	2.4	8	1.8	9	1.25	1000	2.5	0.6	1	0	8.3	5.86	4.75	67.3	

HORIZONTAL TABLE: ALGORITHM 10/7/93, DEFAULT HV TO 0 FOR MISSING DATA

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
Bis(2-ethylhexyl) adipate	5.9	9110	0	-99	0	0	1	0.35	5	0.02	5	9	1.25	1000	2.5	4.2	2.5	0	1	10	6.25	68.8	I
Cyclohexane	3.4	29820	0	500	2.6	0	0	5	3.9	0.39	4	502	2.5	1000	2.5	2.3	1.67	0	2.6	7.92	6.67	70.2	
1,2-Dichloroethane	1.5	780	1.3	2063	1.4	3.5	4	136	1.4	34	0.8	508	2.5	30	1.63	0.6	1	0	10.22	3.57	5.13	70.7	
Cumene	3.7	2910	0.4	8000	0.2	0	2	6	3.7	0.49	3.8	502	2.5	1000	2.5	2.5	1.77	0	2.59	7.9	6.77	71	
Ethylene oxide	-0.3	270	2.1	835	2.2	4	5	474	0.5	118	0	510	2.5	12	1	-1.1	1	2	13.27	2.65	4.5	71.7	
Chlorine	0	8910	0	34	4.9	0	1	0.34	5	0.02	5	9999	2.5	1	1	1	1	0	5.93	10	4.5	71.7	K
Methyl Parathion	3.2	14	4.3	3	5	0	0	9	3.4	0.88	3.4	0	1	1000	1	2.1	1.54	2	9.25	11.1	3.54	72	
Vinylidene chloride	1.8	200	2.3	6350	0.4	1.5	3	108	1.6	27	0.9	503	2.5	1000	2.5	0.9	1	0	7.22	4.89	6	72.7	
Dichlorobenzene (mixed isomers)	3.4	2600	0.5	1100	1.9	0	1	0.54	5	0.05	5	6	1.13	1000	2.5	2.3	1.65	0	3.39	10.47	5.27	73.1	
Ammonia	-0.8	350	1.9	2377	1.2	0	1	2	4.6	0.09	5	9	1.25	1000	2.5	-1.2	1	1	4.17	11.5	4.75	74.5	
1,2-Dichlorobenzene	3.4	1400	0.9	1700	1.5	0	1	0.55	5	0.05	5	6	1.13	1000	2.5	2.3	1.64	0	3.46	10.92	5.27	75.8	
Sulfuric acid	-1.1	2140	0.6	14	5	0	1	31	2.5	2	3	9999	2.5	1000	2.5	-1.3	1	1	6.61	6.14	6	76.6	
4,4'-Methylenedianiline	1.6	185	2.4	163	3.6	3.5	1	45	2.2	11	1.6	8	1.22	1000	2.5	0.7	1	0	10.46	6.2	4.72	78.6	
Trichloroethylene	2.3	2402	0.5	8450	0.1	3.5	4	44	2.3	8	1.8	503	2.5	1000	2.5	1.3	1.15	0	8.18	4.62	6.15	78.7	
Captan	1.8	7500	0	168	3.5	0	4	0.2	5	0.05	5	503	2.5	30	1	0.9	1	2	7.55	10	4.5	79	
Titanium tetrachloride	0	1000	1.2	7	5	0	0	25	2.7	1	3.2	9999	2.5	9999	2.5	-99	1	1	6.17	7.01	6	79	Kc
Hexachloroethane	3.3	4970	0	10000	0	1.5	3	1	4.8	0.13	4.8	503	2.5	30	1.63	2.2	1.59	0	4.5	9.56	5.71	80.3	
Nitric acid	0.2	500	1.7	65	4.4	0	0	26	2.6	1	3.1	9999	2.5	1000	2.5	-0.3	1	1	6.04	7.45	6	81	
4-nitrophenol	0.8	620	1.5	50	4.6	0	2	41	2.3	10	1.6	550	2.5	1000	2.5	-0.1	1	0	8.11	5.47	6	81.5	
1,1,2-Trichloroethane	2.2	150	2.5	2000	1.4	1.5	1	7	3.6	1	3.1	503	2.5	30	1.63	1.2	1.09	0	6.44	9.24	5.22	81.8	
Acrylamide	-0.7	107	2.8	1000	2	3.5	4	109	1.6	27	0.9	9	1.25	360	2.4	-1.4	1	0	12.28	5.33	4.65	81.9	
N-nitrosodiphenylamine	3.1	1650	0.8	-99	0	3.5	1	1	4.8	0.13	4.8	8	1.22	1000	2.5	2.1	1.53	1	5.3	10.45	5.25	82.6	I
Chloroprene	1.4	260	2.1	3253	1	0	5	2	4.4	0.56	3.8	503	2.5	2	1	0.5	1	0	8.12	10.32	4.5	83	
Chlorpyrifos	5	151	2.5	-99	0	0	0	2	4.4	0.12	4.9	503	2.5	1000	1	3.7	2.35	2	2.53	11.77	5.85	83.7	I
Vinyl chloride	1.5	500	1.7	100	4	5	4	143	1.4	36	0.7	6	1.13	1000	2.5	0.6	1	0	14.67	3.82	4.63	85.5	
Tetrachloroethylene	2.6	8100	0	5200	0.6	3.5	4	17	3	2	2.7	503	2.5	1000	2.5	1.6	1.29	0	8.07	5.67	6.29	86.4	
Naphthalene	3.2	2200	0.6	30	5	1	2	6	3.7	0.59	3.7	9	1.23	1000	2.5	2.1	1.56	0	8.59	7.99	5.3	87.9	
1,3-butadiene	2	3210	0.3	128850	0	3.5	4	4	4	1	3.3	502	2.5	1000	2.5	1	1.01	0	7.82	7.62	6.01	92.8	
2,4-Dinitrotoluene	2	268	2.1	-99	0	3.5	3	24	2.7	6	2	550	2.5	1000	2.5	1	1.01	0	8.62	6.84	6.01	92.8	I
Dibutyl phthalate	4.9	9000	0	500	2.6	0	3	1	5	0.05	5	9	1.23	400	2.43	3.6	2.31	0	5.6	9.98	5.98	93.1	
Styrene	3	1000	1.2	2528	1.2	3.5	3	4	4	0.44	3.9	10	1.27	1000	2.5	1.9	1.45	0	8.86	9.08	5.22	93.6	
Hydrogen cyanide	0	4	5	18	5	0	1	1385	0	346	0	9999	2.5	1000	2.5	-0.7	1	0	11	5	6	96	
Copper cmpds	0	300	2	-99	0	0	2	0.33	5	0.02	5	9999	2.5	9999	2.5	-1	1	0	4.04	12.04	6	96.4	KI
Biphenyl	4	3280	0.3	25	5	0	2	2	4.6	0.12	4.9	9	1.23	1000	2.5	2.8	1.9	0	7.31	9.82	5.64	96.5	
Decabromodiphenyl oxide	5.2	2570	0.5	-99	0	0	2	0.06	5	0	5	550	2.5	1000	2.5	3.9	2.44	0	2.48	10.48	7.44	96.5	I
Epichlorohydrin	0.3	40	3.5	500	2.6	3.8	4	35	2.4	9	1.8	510	2.5	30	1	-0.5	1	2	13.85	7.68	4.5	96.9	
1,3-dichloropropene	2	140	2.6	996	2	3.5	1	0.24	5	0.06	5	508	2.5	2	1	1	1	1	9.09	12.59	4.5	97.6	
2,4-Dinitrophenol	1.5	30	3.7	-99	0	0	3	11	3.3	3	2.6	550	2.5	1000	2.5	0.6	1	0	6.7	9.56	6	97.6	I
2,4-D	3.5	275	2.1	-99	0	3.5	3	71	1.9	6	2.1	503	2.5	1000	2.5	2.4	1.71	0	8.6	6.07	6.71	98.5	I
Chlorothalonil	5	6000	0	7	5	0	2	0.05	5	0	5	550	2.5	1	1	3.7	2.36	0	7	10	5.86	99.6	
Di(2-ethylhexyl) phthalate	4.9	30000	0	-99	0	3.5	4	1	4.7	0.08	5	9	1.23	400	2.43	3.6	2.31	0	7.5	9.72	5.97	102.9	I
Hydrogen fluoride	0	50	3.3	86	4.1	0	4	265	1	13	1.5	9999	2.5	1000	2.5	-0.4	1	0	11.47	5.76	6	103.4	
Diaminotoluene (mixed isomers)[24]	1.4	260	2.1	100	4	3.5	2	37	2.4	9	1.7	550	2.5	1000	2.5	0.5	1	0	11.64	6.25	6	107.4	
Anthracene	4.5	17000	0	250	3.2	1	1	0.01	5	0	5	502	2.5	1000	2.5	3.2	2.12	0	5.2	10	7.12	108.3	
Nickel cmpds	0	350	1.9	-99	0	5	3	27	2.6	1	3.1	9999	2.5	9999	2.5	1.6	1.3	0	9.93	7.68	6.3	110.9	KI
Lead cmpds	0	1500	0.9	-99	0	3.5	4	5	3.8	0.26	4.3	9999	2.5	9999	2.5	1.8	1.39	0	8.37	9.01	6.39	111.1	KI
Cobalt cmpds	0	55	3.3	-99	0	0	1	0.38	5	0.02	5	9999	2.5	9999	2.5	1.7	1.35	0	4.26	13.26	6.35	111.3	KI
Formaldehyde	1.1	260	2.1	480	2.6	4	3	24	2.7	6	2	502	2.5	1000	2.5	0.2	1	0	11.78	6.87	6	111.9	
2-nitropropane	1.1	725	1.4	600	2.4	3.5	3	5	3.9	1	3.2	550	2.5	1000	2.5	0.2	1	0	10.34	8.49	6	113	
Chromium cmpds	0	97	2.9	-99	0	5	1	33	2.5	2	3	9999	2.5	9999	2.5	2.3	1.65	0	8.85	8.29	6.65	114	KI

HORIZONTAL TABLE: ALGORITHM 10/7/93, DEFAULT HV TO 0 FOR MISSING DATA

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	env	mult	sum	bad (a)
1,2,4-Trichlorobenzene	4	300	2	1100	1.9	0	2	3	4.2	0.2	4.5	550	2.5	1000	2.5	2.9	1.93	0	5.95	10.73	6.93	115.7	
Hexachlorobenzene	4.1	4000	0.2	306	3	3.5	4	22	2.8	1	3.1	550	2.5	1000	2.5	3	1.98	0	10.68	5.99	6.98	116.5	
Trifluralin	3.1	500	1.7	47	4.7	0	3	0.11	5	0.01	5	503	2.5	30	1.63	2	1.5	0	9.33	11.67	5.82	118.1	
Polychlorinated biphenyls	6.3	1300	1	-99	0	3.8	3	3	4.3	0.14	4.8	550	2.5	1000	2.5	4.2	2.5	0	7.73	10.02	7.5	133.1	I
Hexachloro-1,3-butadiene	4.9	102	2.8	35	4.9	1.5	3	0.09	5	0	5	503	2.5	2	1	3.6	2.31	0	12.23	12.82	5.81	145.6	
Terbufos (tBuSCH2SP(=S)(OEt)2	4.5	3	5	1	5	0	0	0.01	5	0	5	508	2.5	15	1.41	3.3	2.15	1	10	15	6.06	151.6	
Arsenic cmpds	0	8	4.7	-99	0	5	3	32	2.5	2	3	9999	2.5	9999	2.5	2.5	1.75	1	12.66	10.14	6.75	153.9	KI
Cadmium cmpds	0	88	2.9	306	3	4	3	0.1	5	0	5	9999	2.5	9999	2.5	3.5	2.25	0	12.95	12.92	7.25	187.6	K

(a): Missing/no QSAR: I=inhl, O=oral, N=Fish Noefft, F=Fish, K=logKow, b=BOD, h=Hydro, c=log BCF

HORIZONTAL TABLE: 10/8/93 ALGORITHM, DEFAULT HV TO 5 FOR MISSING DATA

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
sec-butyl alcohol	0.6	6480	0	8000	0.2	0	0	3670	0	918	0	9	1.25	1000	2.5	-0.2	1	0	0.19	0	4.75	0.9	
Methyl tert-butyl ether	0.9	4000	0.2	23568	0	0	0	786	0.2	197	0	508	2.5	1000	2.5	0	1	0	0.16	0.34	6	3	
tert-butyl alcohol	0.4	3500	0.3	8000	0.2	0	0	1954	0	488	0	508	2.5	1000	2.5	-0.5	1	0	0.45	0.26	6	4.3	
Methanol	-0.6	5628	0	64000	0	0	1	29400	0	7350	0	9	1.25	1000	2.5	-1.4	1	0	1	0	4.75	4.8	
Carbonyl sulfide	0.1	0	0	10000	0	0	1	2685	0	671	0	9,999	2.5	1000	2.5	-0.7	1	0	1	0	6	6	
Acetone	-0.2	3000	0.4	42000	0	0	1	7200	0	1800	0	7	1.15	1000	2.5	-1	1	0	1.37	0.37	4.65	8.1	
Acetonitrile	-0.3	3800	0.2	15000	0	0	3	1640	0	410	0	5	1.07	1	1	-1.1	1	0	3.2	0.2	3.07	10.4	
Freon 113	1.7	43000	0	10000	0	0	1	290	0.9	73	0.2	503	2.5	30	1.63	0.7	1	0	1	1.13	5.13	10.9	
Ethylene glycol	-1.9	6610	0	1000	2	0	1	227634	0	56909	0	9	1.25	1000	2.5	-2.5	1	0	3	0	4.75	14.3	
Aluminum (fume or dust)	0	9999	0	500	2.6	0	0	-99	0	-99	0	500	2.5	9999	2.5	-99	1	0	2.6	0	6	15.6	KFNc
n-butyl alcohol	0.9	790	1.3	8000	0.2	0	1	1860	0	465	0	9	1.25	1000	2.5	0	1	0	2.53	1.34	4.75	18.4	
Methyl isobutyl ketone	1.2	2080	0.6	5672	0.5	0	2	505	0.5	126	0	7	1.15	1000	2.5	0.3	1	0	3.13	1.13	4.65	19.8	
1,2-Dichloropropane	2.3	3000	0.4	5554	0.5	0	0	127	1.5	23	1.1	503	2.5	30	1.63	1.3	1.14	0	0.88	2.92	5.27	20	
Methyl methacrylate	1.4	8000	0	7500	0.2	0	3	259	1	65	0.3	9	1.25	1000	2.5	0.5	1	0	3.25	1.29	4.75	21.6	
Glycol ethers	0.8	1200	1	450	2.7	0	0	1490	0	373	0	9	1.25	1000	2.5	0	1	0	3.73	1.03	4.75	22.6	
Methyl ethyl ketone	0.3	2737	0.4	6766	0.3	0	4	3220	0	805	0	7	1.15	1000	2.5	-0.5	1	0	4.78	0.44	4.65	24.2	
Glyphosate	-3.3	4873	0	-99	5	0	0	600	0.4	150	0	9	1.25	1000	2.5	-3.7	1	0	5.02	0.39	4.75	25.7	I
Butyraldehyde	0.9	2490	0.5	7547	0.2	0	0	32	2.5	8	1.8	7	1.15	1000	2.5	0	1	1	0.75	4.82	4.65	25.9	
Diethanolamine	-1.4	710	1.4	484	2.6	0	0	4710	0	1178	0	9	1.25	1000	2.5	-2.1	1	0	4.04	1.41	4.75	25.9	
1,4-Dioxane	-0.3	3150	0.3	6368	0.4	3.5	0	10352	0	2588	0	520	2.5	1000	2.5	-1	1	0	4.23	0.33	6	27.4	
Phthalic anhydride	1.3	2000	0.7	1000	2	0	2	364	0.7	91	0.1	550	2.5	1000	1	0.4	1	2	4.66	1.46	4.5	27.6	
2-ethoxyethanol	-0.5	1400	0.9	3185	1	0	3	16305	0	4076	0	9	1.25	1000	2.5	-1.3	1	0	4.92	0.92	4.75	27.7	
Chloromethane	0.9	1800	0.7	3063	1	1.5	3	550	0.4	138	0	6	1.13	30	1.63	0	1	0	6.27	1.17	3.75	27.9	
Dimethyl phthalate	1.3	2400	0.5	500	2.6	0	0	121	1.5	30	0.9	9	1.25	400	2.43	0.4	1	0	3.13	2.93	4.68	28.4	
Isobutyraldehyde	0.6	2810	0.4	6681	0.4	0	1	41	2.3	10	1.6	7	1.15	1000	2.5	-0.2	1	1	1.77	4.37	4.65	28.6	
Vinyl acetate	0.7	1613	0.8	3680	0.9	0	1	100	1.7	25	1	9	1.25	1000	2.5	-0.1	1	0	2.69	3.49	4.75	29.4	
Zinc (fume or dust)	0	9999	0	1000	2	0	3	-99	0	-99	0	500	2.5	9999	2.5	-2	1	0	5	0	6	30	KFN
Maleic anhydride	0.1	465	1.7	1000	2	3	1	2963	0	741	0	8	1.2	1000	1	-0.7	1	2	7.72	1.72	3.2	30.2	
2-methoxyethanol	-0.8	950	1.2	2590	1.2	0	3	22655	0	5664	0	9	1.25	1000	2.5	-1.5	1	0	5.38	1.2	4.75	31.3	
Ethylene	1.1	9999	0	950000	0	0	1	14	3.1	3	2.4	10	1.28	1000	2.5	0.2	1	0	1	5.55	4.78	31.4	
Propylene	1.8	9999	0	10500	0	0	0	5	3.8	1	3.2	10	1.28	1000	2.5	0.8	1	0	0	6.97	4.78	33.4	
Ammonium sulfate (solution)	0	3000	0.4	-99	5	0	0	4000	0	200	0	9,999	2.5	9999	2.5	-2	1	0	5.37	0.37	6	34.4	KI
Pyridine	0.6	1580	0.8	1000	2	0	1	100	1.7	25	1	9	1.23	1000	2.5	-0.2	1	0	3.83	3.51	4.73	34.7	
Diethyl phthalate	2.5	9000	0	537	2.5	0	0	32	2.5	5	2.2	9	1.25	400	2.43	1.5	1.23	0	2.54	4.68	4.91	35.5	
Isopropyl alcohol	0.3	3600	0.2	32000	0	5	2	8623	0	2156	0	9	1.25	1000	2.5	-0.5	1	0	7.24	0.24	4.75	35.5	
Toluene	2.7	5050	0	6675	0.4	0	2	34	2.4	4	2.3	10	1.27	1000	2.5	1.7	1.33	0	2.35	4.7	5.1	36	
Asbestos (friable)	0	9999	0	9999	0	5	1	-99	0	-99	0	9,999	2.5	9999	2.5	1	1	0	6	0	6	36	KFN
Dichloromethane	1.3	1600	0.8	17400	0	3.5	1	330	0.8	83	0.1	508	2.5	30	1.63	0.4	1	0	5.32	1.77	5.13	36.4	
Benzoyl chloride	2.2	2460	0.5	163	3.6	0	2	35	2.4	7	1.9	9	1.25	1000	1	1.2	1.12	2	6.09	4.89	3.37	37	
Chloroethane	1.4	7500	0	29	5	0	0	16	3	4	2.3	6	1.13	30	1.63	0.5	1	0	5	5.29	3.75	38.6	
Carbon disulfide	0.8	2780	0.4	1604	1.6	0	4	694	0.3	174	0	9,999	2.5	1000	2.5	0	1	0	6.01	0.69	6	40.2	
Allyl chloride	-0.2	425	1.8	926	2.1	1.5	3	72	1.9	18	1.2	6	1.13	2	1	-1	1	0	8.35	4.92	3.13	41.5	
Ammonium nitrate (solution)	0	4500	0.1	-99	5	0	1	800	0.2	40	0.7	9,999	2.5	9999	2.5	-2	1	0	6.08	0.9	6	41.9	KI
Thorium dioxide	0	1140	1.1	-99	5	0	0	-99	0	-99	0	9,999	2.5	9999	2.5	-99	1	0	6.07	1.07	6	42.8	KIFNc
Butyl acrylate	2.4	3730	0.2	2730	1.1	0	0	2	4.6	0.31	4.2	9	1.25	50	1.78	1.4	1.18	0	1.34	8.94	4.22	43.3	
Acrylic acid	0.4	193	2.4	1200	1.8	0	1	186	1.2	47	0.6	8	1.2	1000	2.5	-0.5	1	0	5.2	4.13	4.7	43.8	
EPTC (ethyl dipropylthiocarbamate)	3.2	916	1.2	4062	0.8	0	0	27	2.6	3	2.6	9	1.25	1000	2.5	2.1	1.56	1	2.01	6.48	5.31	45.1	
1,1,1-Trichloroethane	2.5	11240	0	2000	1.4	0	3	48	2.2	7	1.9	503	2.5	30	1.63	1.5	1.24	0	4.4	4.11	5.37	45.6	
m-Xylene	3.2	5000	0	4550	0.7	0	2	16	3	2	3	10	1.27	1000	2.5	2.1	1.56	0	2.68	6.01	5.33	46.4	
Propylene oxide	0	690	1.4	1740	1.5	4	5	306	0.9	77	0.2	9	1.25	1000	1	-0.8	1	2	11.95	2.48	3.25	46.9	

HORIZONTAL TABLE: 10/8/93 ALGORITHM, DEFAULT HV TO 5 FOR MISSING DATA

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
Carbaryl	2.4	500	1.7	25000	0	0	4	8	3.5	1	3.2	8	1.22	1000	1	1.4	1.16	2	5.67	8.35	3.4	47.6	
Metribuzin	1.7	7500	0	-99	5	0	0	80	1.8	20	1.2	508	2.5	1000	2.5	0.8	1	0	5	2.99	6	48	I
o-Xylene	2.8	5000	0	4550	0.7	0	3	16	3	2	2.8	10	1.27	1000	2.5	1.7	1.37	0	3.68	5.8	5.14	48.7	
Antimony cmpds	0	20000	0	-99	5	0	2	833	0.1	42	0.6	9,999	2.5	9999	2.5	1.6	1.3	0	7	0.77	6.3	48.9	KI
Propionaldehyde	0.3	1200	1	4581	0.7	3	1	44	2.3	11	1.6	7	1.15	1000	2.5	-0.5	1	1	5.71	4.9	4.65	49.4	
Acetaldehyde	-0.2	1930	0.7	1500	1.6	3.5	0	34	2.4	9	1.8	7	1.15	1000	2.5	-1	1	1	5.84	4.92	4.65	50	
Xylene (mixed isomers)	3	4300	0.1	6350	0.4	0	3	13	3.1	1	3.1	10	1.27	1000	2.5	1.9	1.47	0	3.5	6.3	5.24	51.4	
Aniline	0.9	250	2.2	306	3	0	1	108	1.6	27	0.9	9	1.25	1000	2.5	0	1	0	6.2	4.73	4.75	51.9	
Methylenebis(phenylisocyanate)	3.4	2200	0.6	5	5	0	0	66	2	6	2.1	550	2.5	1000	1	2.3	1.64	2	5.59	4.62	5.14	52.6	
1,2,4-Trimethylbenzene	3.4	5000	0	3655	0.9	0	0	8	3.5	0.68	3.6	502	2.5	1000	2.5	2.3	1.65	0	0.87	7.14	6.65	53.3	
Metam Sodium (MeNHCS2Na)	1	285	2.1	888	2.1	0	0	0.39	5	0.1	5	10	1.28	1	1	0.1	1	1	4.18	12.07	3.28	53.4	
Ethylbenzene	3.2	5460	0	5000	0.6	0	3	11	3.3	1	3.3	10	1.27	1000	2.5	2.1	1.54	0	3.6	6.59	5.31	54.1	
Bromomethane	1.2	214	2.3	780	2.2	0	2	11	3.3	3	2.6	6	1.13	30	1.63	0.3	1	0	6.5	8.15	3.75	54.9	
Maneb	0	4400	0.1	-99	5	0	4	2	4.6	0.09	5	(99)	1	-99	1	-99	1	0	9.09	9.67	3	56.3	Klbhc
N,N-Dimethylaniline	2.3	1410	0.9	1225	1.8	0	2	65	2	12	1.6	513	2.5	1000	2.5	1.3	1.16	0	4.74	4.45	6.16	56.6	
Cumene hydroperoxide	2.3	382	1.9	200	3.4	1	0	62	2	11	1.6	9	1.23	1000	2.5	1.3	1.14	0	6.26	5.45	4.87	57	
Cyanazine	1.9	261	2.1	230	3.3	0	0	18	2.9	5	2.2	503	2.5	1	1	0.9	1	2	5.41	7.29	4.5	57.2	
Chlorobenzene	2.8	1440	0.9	1100	1.9	0	2	17	3	2	2.8	6	1.13	1000	2.5	1.8	1.4	0	4.82	6.69	5.02	57.8	
Hydroquinone	0.6	320	2	-99	5	0	1	141	1.4	35	0.8	9	1.25	1000	2.5	-0.2	1	0	7.99	4.17	4.75	57.8	I
Nitrobenzene	1.9	640	1.5	-99	5	0	2	119	1.5	30	0.9	9	1.23	1000	2.5	0.9	1	0	8.49	3.91	4.73	58.7	I
Toluene-2,4-diisocyanate	1.8	5800	0	10	5	3.5	1	53	2.1	13	1.5	550	2.5	1000	1	0.8	1	2	9.5	3.6	4.5	58.9	
Atrazine	2.3	1750	0.8	540	2.5	0	0	16	3	3	2.6	503	2.5	1000	2.5	1.3	1.17	0	3.3	6.35	6.17	59.5	
Chlorine dioxide	0	292	2.1	130	3.8	0	2	0.17	5	0.01	5	5	1.07	1	1	-99	1	0	7.83	12.06	3.07	61	Kc
Hydrochloric acid	1.1	900	1.2	277	3.1	0	1	19	2.9	0.95	3.4	10	1.28	1000	2.5	0.5	1	1	5.36	7.48	4.78	61.4	
p-Xylene	3.2	5000	0	4550	0.7	0	2	2	4.5	0.2	4.5	10	1.27	1000	2.5	2.1	1.54	0	2.68	9	5.31	62	
1,4-Dichlorobenzene	3.4	3790	0.2	1100	1.9	3.5	1	34	2.5	3	2.5	6	1.13	1000	2.5	2.3	1.65	0	6.62	5.2	5.27	62.3	
Metolachlor	3.5	2780	0.4	-99	5	0	0	15	3	1	3.2	503	2.5	2	1	2.4	1.68	2	5.43	6.62	5.18	62.3	I
Terephthalic acid	1.6	18800	0	-99	5	0	1	29	2.6	7	1.9	550	2.5	1000	2.5	0.7	1	0	6	4.45	6	62.7	I
Benzene	2.1	4700	0	17500	0	5	3	19	2.9	4	2.3	10	1.27	1000	2.5	1.2	1.08	0	8.04	5.26	4.84	64.5	
Chloroform	2	908	1.2	5720	0.5	3.5	3	71	1.9	18	1.3	503	2.5	30	1.63	1	1	0	8.22	4.41	5.13	64.8	
Chlorophenols [o]	2.3	261	2.1	100	4	0	0	19	2.9	3	2.4	6	1.13	1000	2.5	1.3	1.15	0	6.14	7.45	4.78	64.9	
4,4'-Isopropylidenediphenol	3.3	2500	0.5	200	3.4	0	0	5	3.9	0.42	4	8	1.2	1000	2.5	2.2	1.62	0	3.9	8.36	5.31	65.1	
Carbon tetrachloride	2.8	2800	0.4	19052	0	3.5	3	41	2.3	5	2.2	503	2.5	30	1.63	1.8	1.39	0	6.92	4.9	5.52	65.3	
Butylate	3.7	4659	0.1	-99	5	0	0	7	3.6	0.54	3.8	518	2.5	1000	1	2.5	1.77	2	5.05	7.43	5.27	65.7	I
p-Cresol	2	207	2.3	50	4.6	0	0	25	2.7	6	2	9	1.23	1000	2.5	1	1	0	6.91	6.98	4.73	65.8	
Acrylonitrile	-0.9	78	3	576	2.5	4	3	10	3.3	3	2.7	5	1.07	1	1	-1.6	1	0	12.49	9	3.07	66	
Cresol (mixed isomers)	2	760	1.4	50	4.6	0	1	13	3.2	3	2.5	9	1.23	1000	2.5	1	1	0	6.97	7.01	4.73	66.2	
Malathion	2.9	570	1.6	6	5	0	0	0.1	5	0.01	5	9	1.25	1000	1	1.8	1.4	2	6.57	11.57	3.66	66.3	
Phosphoric acid	-0.6	1530	0.9	14	5	0	0	70	1.9	4	2.4	9,999	2.5	1000	2.5	-0.9	1	1	5.86	5.21	6	66.4	
Phenol	1.5	530	1.6	46	4.7	0	2	34	2.4	8	1.8	9	1.25	1000	2.5	0.6	1	0	8.3	5.86	4.75	67.3	
Cyclohexane	3.4	29820	0	500	2.6	0	0	5	3.9	0.39	4	502	2.5	1000	2.5	2.3	1.67	0	2.6	7.92	6.67	70.2	
1,2-Dichloroethane	1.5	780	1.3	2063	1.4	3.5	4	136	1.4	34	0.8	508	2.5	30	1.63	0.6	1	0	10.22	3.57	5.13	70.7	
Cumene	3.7	2910	0.4	8000	0.2	0	2	6	3.7	0.49	3.8	502	2.5	1000	2.5	2.5	1.77	0	2.59	7.9	6.77	71	
Butyl benzyl phthalate	4.8	2330	0.6	-99	5	0	1	43	2.3	2	2.7	8	1.2	400	2.43	3.5	2.26	0	6.55	5.56	5.89	71.3	I
Ethylene oxide	-0.3	270	2.1	835	2.2	4	5	474	0.5	118	0	510	2.5	12	1	-1.1	1	2	13.27	2.65	4.5	71.7	
Chlorine	0	8910	0	34	4.9	0	1	0.34	5	0.02	5	9,999	2.5	1	1	1	1	0	5.93	10	4.5	71.7	K
Methyl Parathion	3.2	14	4.3	3	5	0	0	9	3.4	0.88	3.4	0	1	1000	1	2.1	1.54	2	9.25	11.1	3.54	72	
Vinylidene chloride	1.8	200	2.3	6350	0.4	1.5	3	108	1.6	27	0.9	503	2.5	1000	2.5	0.9	1	0	7.22	4.89	6	72.7	
Dichlorobenzene (mixed isomers)	3.4	2600	0.5	1100	1.9	0	1	0.54	5	0.05	5	6	1.13	1000	2.5	2.3	1.65	0	3.39	10.47	5.27	73.1	
Catechol	0.9	260	2.1	-99	5	0	0	9	3.4	2	2.7	9	1.25	1000	2.5	0	1	0	7.14	8.26	4.75	73.2	I

HORIZONTAL TABLE: 10/8/93 ALGORITHM, DEFAULT HV TO 5 FOR MISSING DATA

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
Ammonia	-0.8	350	1.9	2377	1.2	0	1	2	4.6	0.09	5	9	1.25	1000	2.5	-1.2	1	1	4.17	11.5	4.75	74.5	
Alachlor	3.1	1065	1.1	-99	5	0	0	5	3.8	0.51	3.8	503	2.5	2	1	2	1.51	2	6.12	8.77	5.01	74.7	I
1,2-Dichlorobenzene	3.4	1400	0.9	1700	1.5	0	1	0.55	5	0.05	5	6	1.13	1000	2.5	2.3	1.64	0	3.46	10.92	5.27	75.8	
Sulfuric acid	-1.1	2140	0.6	14	5	0	1	31	2.5	2	3	9,999	2.5	1000	2.5	-1.3	1	1	6.61	6.14	6	76.6	
4,4'-Methylenedianiline	1.6	185	2.4	163	3.6	3.5	1	45	2.2	11	1.6	8	1.22	1000	2.5	0.7	1	0	10.46	6.2	4.72	78.6	
Trichloroethylene	2.3	2402	0.5	8450	0.1	3.5	4	44	2.3	8	1.8	503	2.5	1000	2.5	1.3	1.15	0	8.18	4.62	6.15	78.7	
Captan	1.8	7500	0	168	3.5	0	4	0.2	5	0.05	5	503	2.5	30	1	0.9	1	2	7.55	10	4.5	79	
Titanium tetrachloride	0	1000	1.2	7	5	0	0	25	2.7	1	3.2	9,999	2.5	9999	2.5	-99	1	1	6.17	7.01	6	79	Kc
Zinc compounds	0	7950	0	-99	5	0	0	17	2.9	0.86	3.4	9,999	2.5	9999	2.5	3	2	0	5	6.39	7	79.7	Kl
Hexachloroethane	3.3	4970	0	10000	0	1.5	3	1	4.8	0.13	4.8	503	2.5	30	1.63	2.2	1.59	0	4.5	9.56	5.71	80.3	
Nitric acid	0.2	500	1.7	65	4.4	0	0	26	2.6	1	3.1	9,999	2.5	1000	2.5	-0.3	1	1	6.04	7.45	6	81	
Phosphorus (yellow or white)	3	3	5	-99	5	0	2	0.02	5	0	5	(99)	1	0	1	1	1	0	12	15	3	81	Ib
4-nitrophenol	0.8	620	1.5	50	4.6	0	2	41	2.3	10	1.6	550	2.5	1000	2.5	-0.1	1	0	8.11	5.47	6	81.5	
1,1,2-Trichloroethane	2.2	150	2.5	2000	1.4	1.5	1	7	3.6	1	3.1	503	2.5	30	1.63	1.2	1.09	0	6.44	9.24	5.22	81.8	
Acrylamide	-0.7	107	2.8	1000	2	3.5	4	109	1.6	27	0.9	9	1.25	360	2.4	-1.4	1	0	12.28	5.33	4.65	81.9	
Chloroprene	1.4	260	2.1	3253	1	0	5	2	4.4	0.56	3.8	503	2.5	2	1	0.5	1	0	8.12	10.32	4.5	83	
Vinyl chloride	1.5	500	1.7	100	4	5	4	143	1.4	36	0.7	6	1.13	1000	2.5	0.6	1	0	14.67	3.82	4.63	85.5	
Manganese cmpds	0	615	1.5	-99	5	0	3	150	1.4	8	1.9	9,999	2.5	9999	2.5	1	1	0	9.52	4.77	6	85.7	Kl
Molybdenum trioxide	0	125	2.7	-99	5	0	2	370	0.7	19	1.2	9,999	2.5	9999	2.5	-99	1	0	9.67	4.61	6	85.7	Klc
Tetrachloroethylene	2.6	8100	0	5200	0.6	3.5	4	17	3	2	2.7	503	2.5	1000	2.5	1.6	1.29	0	8.07	5.67	6.29	86.4	
Picric acid	2	30	3.7	-99	5	0	0	170	1.3	41	0.6	550	2.5	1000	2.5	1.1	1.03	0	8.7	5.63	6.03	86.5	I
Naphthalene	3.2	2200	0.6	30	5	1	2	6	3.7	0.59	3.7	9	1.23	1000	2.5	2.1	1.56	0	8.59	7.99	5.3	87.9	
Barium cmpds	0	132	2.6	-99	5	0	2	200	1.2	10	1.7	9,999	2.5	9999	2.5	1	1	0	9.63	5.46	6	90.6	Kl
1,3-butadiene	2	3210	0.3	128850	0	3.5	4	4	4	1	3.3	502	2.5	1000	2.5	1	1.01	0	7.82	7.62	6.01	92.8	
Dibutyl phthalate	4.9	9000	0	500	2.6	0	3	1	5	0.05	5	9	1.23	400	2.43	3.6	2.31	0	5.6	9.98	5.98	93.1	
Styrene	3	1000	1.2	2528	1.2	3.5	3	4	4	0.44	3.9	10	1.27	1000	2.5	1.9	1.45	0	8.86	9.08	5.22	93.6	
Hydrogen cyanide	0	4	5	18	5	0	1	1385	0	346	0	9,999	2.5	1000	2.5	-0.7	1	0	11	5	6	96	
Biphenyl	4	3280	0.3	25	5	0	2	2	4.6	0.12	4.9	9	1.23	1000	2.5	2.8	1.9	0	7.31	9.82	5.64	96.5	
Epichlorohydrin	0.3	40	3.5	500	2.6	3.8	4	35	2.4	9	1.8	510	2.5	30	1	-0.5	1	2	13.85	7.68	4.5	96.9	
1,3-dichloropropene	2	140	2.6	996	2	3.5	1	0.24	5	0.06	5	508	2.5	2	1	1	1	1	9.09	12.59	4.5	97.6	
Di-n-octyl phthalate	5.2	13000	0	-99	5	0	1	0.93	5	0.05	5	9	1.23	400	2.43	3.9	2.44	0	6	10	6.1	97.6	I
Chlorothalonil	5	6000	0	7	5	0	2	0.05	5	0	5	550	2.5	1	1	3.7	2.36	0	7	10	5.86	99.6	
Bis(2-ethylhexyl) adipate	5.9	9110	0	-99	5	0	1	0.35	5	0.02	5	9	1.25	1000	2.5	4.2	2.5	0	6	10	6.25	100	I
Hydrogen fluoride	0	50	3.3	86	4.1	0	4	265	1	13	1.5	9,999	2.5	1000	2.5	-0.4	1	0	11.47	5.76	6	103.4	
Diaminotoluene (mixed isomers)[24]	1.4	260	2.1	100	4	3.5	2	37	2.4	9	1.7	550	2.5	1000	2.5	0.5	1	0	11.64	6.25	6	107.4	
Anthracene	4.5	17000	0	250	3.2	1	1	0.01	5	0	5	502	2.5	1000	2.5	3.2	2.12	0	5.2	10	7.12	108.3	
N-nitrosodiphenylamine	3.1	1650	0.8	-99	5	3.5	1	1	4.8	0.13	4.8	8	1.22	1000	2.5	2.1	1.53	1	10.3	10.45	5.25	108.9	I
Formaldehyde	1.1	260	2.1	480	2.6	4	3	24	2.7	6	2	502	2.5	1000	2.5	0.2	1	0	11.78	6.87	6	111.9	
2-nitropropane	1.1	725	1.4	600	2.4	3.5	3	5	3.9	1	3.2	550	2.5	1000	2.5	0.2	1	0	10.34	8.49	6	113	
Chlorpyrifos	5	151	2.5	-99	5	0	0	2	4.4	0.12	4.9	503	2.5	1000	1	3.7	2.35	2	7.53	11.77	5.85	113	I
1,2,4-Trichlorobenzene	4	300	2	1100	1.9	0	2	3	4.2	0.2	4.5	550	2.5	1000	2.5	2.9	1.93	0	5.95	10.73	6.93	115.7	
Hexachlorobenzene	4.1	4000	0.2	308	3	3.5	4	22	2.8	1	3.1	550	2.5	1000	2.5	3	1.98	0	10.68	5.99	6.98	116.5	
Trifluralin	3.1	500	1.7	47	4.7	0	3	0.11	5	0.01	5	503	2.5	30	1.63	2	1.5	0	9.33	11.67	5.62	118.1	
2,4-Dinitrotoluene	2	268	2.1	-99	5	3.5	3	24	2.7	6	2	550	2.5	1000	2.5	1	1.01	0	13.62	6.84	6.01	122.9	I
Copper cmpds	0	300	2	-99	5	0	2	0.33	5	0.02	5	9,999	2.5	9999	2.5	-1	1	0	9.04	12.04	6	126.4	Kl
2,4-Dinitrophenol	1.5	30	3.7	-99	5	0	3	11	3.3	3	2.6	550	2.5	1000	2.5	0.6	1	0	11.7	9.56	6	127.6	I
2,4-D	3.5	275	2.1	-99	5	3.5	3	71	1.9	6	2.1	503	2.5	1000	2.5	2.4	1.71	0	13.6	6.07	6.71	132	I
Di(2-ethylhexyl) phthalate	4.9	30000	0	-99	5	3.5	4	1	4.7	0.08	5	9	1.23	400	2.43	3.6	2.31	0	12.5	9.72	5.97	132.8	I
Decabromodiphenyl oxide	5.2	2570	0.5	-99	5	0	2	0.06	5	0	5	550	2.5	1000	2.5	3.9	2.44	0	7.48	10.48	7.44	133.7	I
Nickel cmpds	0	350	1.9	-99	5	5	3	27	2.6	1	3.1	9,999	2.5	9999	2.5	1.6	1.3	0	14.93	7.68	6.3	142.4	Kl

HORIZONTAL TABLE: 10/8/93 ALGORITHM, DEFAULT HV TO 5 FOR MISSING DATA

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	nlox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
Lead cmpds	0	1500	0.9	-99	5	3.5	4	5	3.8	0.26	4.3	9,999	2.5	9999	2.5	1.8	1.39	0	13.37	9.01	6.39	143	KI
Cobalt cmpds	0	55	3.3	-99	5	0	1	0.38	5	0.02	5	9,999	2.5	9999	2.5	1.7	1.35	0	9.26	13.26	6.35	143.1	KI
Hexachloro-1,3-butadiene	4.9	102	2.8	35	4.9	1.5	3	0.09	5	0	5	503	2.5	2	1	3.6	2.31	0	12.23	12.82	5.81	145.6	
Chromium cmpds	0	97	2.9	-99	5	5	1	33	2.5	2	3	9,999	2.5	9999	2.5	2.3	1.65	0	13.65	8.29	6.65	147.2	KI
Terbufos (tBuSCH2SP(=S)(OEt)2	4.5	3	5	1	5	0	0	0.01	5	0	5	508	2.5	15	1.41	3.3	2.15	1	10	15	6.06	151.6	
Polychlorinated biphenyls	6.3	1300	1	-99	5	3.8	3	3	4.3	0.14	4.8	550	2.5	1000	2.5	4.2	2.5	0	12.73	10.02	7.5	170.6	I
Cadmium cmpds	0	88	2.9	306	3	4	3	0.1	5	0	5	9,999	2.5	9999	2.5	3.5	2.25	0	12.95	12.92	7.25	187.6	K
Arsenic cmpds	0	8	4.7	-99	5	5	3	32	2.5	2	3	9,999	2.5	9999	2.5	2.5	1.75	1	17.66	10.14	6.75	187.7	KI

(a): Missing/no QSAR: I=inhl, O=oral, N=Fish Noefft, F=Fish, K=logKow, b=BOD, h=Hydro, c=log BCF

HORIZONTAL TABLE: 10/8/93 ALGORITHM, 'OTHER SPECIFIC EFFECTS' EXCLUDED

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
Carbonyl sulfide	0.1	0	0	10000	0	0	0	2685	0	671	0	9999	2.5	1000	2.5	-0.7	1	0	0	0	6	0	
Methanol	-0.6	5628	0	64000	0	0	0	29400	0	7350	0	9	1.25	1000	2.5	-1.4	1	0	0	0	4.75	0	
sec-butyl alcohol	0.6	6480	0	8000	0.2	0	0	3670	0	918	0	9	1.25	1000	2.5	-0.2	1	0	0.19	0	4.75	0.9	
Acetonitrile	-0.3	3800	0.2	15000	0	0	0	1640	0	410	0	5	1.07	1	1	-1.1	1	0	0.2	0.2	3.07	1.2	
Glyphosate	-3.3	4873	0	-99	0	0	0	600	0.4	150	0	9	1.25	1000	2.5	-3.7	1	0	0.02	0.39	4.75	1.9	I
Methyl tert-butyl ether	0.9	4000	0.2	23568	0	0	0	786	0.2	197	0	508	2.5	1000	2.5	0	1	0	0.16	0.34	6	3	
Acetone	-0.2	3000	0.4	42000	0	0	0	7200	0	1800	0	7	1.15	1000	2.5	-1	1	0	0.37	0.37	4.65	3.4	
tert-butyl alcohol	0.4	3500	0.3	8000	0.2	0	0	1954	0	488	0	508	2.5	1000	2.5	-0.5	1	0	0.45	0.26	6	4.3	
Ammonium sulfate (solution)	0	3000	0.4	-99	0	0	0	4000	0	200	0	9999	2.5	9999	2.5	-2	1	0	0.37	0.37	6	4.4	KI
Antimony cmpds	0	20000	0	-99	0	0	0	833	0.1	42	0.6	9999	2.5	9999	2.5	1.6	1.3	0	0	0.77	6.3	4.8	KI
Methyl ethyl ketone	0.3	2737	0.4	6766	0.3	0	0	3220	0	805	0	7	1.15	1000	2.5	-0.5	1	0	0.78	0.44	4.65	5.6	
Freon 113	1.7	43000	0	10000	0	0	0	290	0.9	73	0.2	503	2.5	30	1.63	0.7	1	0	0	1.13	5.13	5.8	
Ammonium nitrate (solution)	0	4500	0.1	-99	0	0	0	800	0.2	40	0.7	9999	2.5	9999	2.5	-2	1	0	0.08	0.9	6	5.9	KI
Methyl methacrylate	1.4	8000	0	7500	0.2	0	0	259	1	65	0.3	9	1.25	1000	2.5	0.5	1	0	0.25	1.29	4.75	7.3	
Ethylene glycol	-1.9	6610	0	1000	2	0	0	227634	0	56909	0	9	1.25	1000	2.5	-2.5	1	0	2	0	4.75	9.5	
Methyl isobutyl ketone	1.2	2080	0.6	5672	0.5	0	0	505	0.5	126	0	7	1.15	1000	2.5	0.3	1	0	1.13	1.13	4.65	10.5	
Zinc (fume or dust)	0	9999	0	1000	2	0	0	-99	0	-99	0	500	2.5	9999	2.5	-2	1	0	2	0	6	12	KFN
Thorium dioxide	0	1140	1.1	-99	0	0	0	-99	0	-99	0	9999	2.5	9999	2.5	-99	1	0	1.07	1.07	6	12.8	KIFNc
2-ethoxyethanol	-0.5	1400	0.9	3185	1	0	0	16305	0	4076	0	9	1.25	1000	2.5	-1.3	1	0	1.92	0.92	4.75	13.5	
n-butyl alcohol	0.9	790	1.3	8000	0.2	0	0	1860	0	465	0	9	1.25	1000	2.5	0	1	0	1.53	1.34	4.75	13.6	
Aluminum (fume or dust)	0	9999	0	500	2.6	0	0	-99	0	-99	0	500	2.5	9999	2.5	-99	1	0	2.6	0	6	15.6	KFNc
Carbon disulfide	0.8	2780	0.4	1604	1.6	0	0	694	0.3	174	0	9999	2.5	1000	2.5	0	1	0	2.01	0.69	6	16.2	
Chloromethane	0.9	1800	0.7	3063	1	1.5	0	550	0.4	138	0	6	1.13	30	1.63	0	1	0	3.27	1.17	3.75	16.7	
2-methoxyethanol	-0.8	950	1.2	2590	1.2	0	0	22655	0	5664	0	9	1.25	1000	2.5	-1.5	1	0	2.38	1.2	4.75	17	
Metribuzin	1.7	7500	0	-99	0	0	0	80	1.8	20	1.2	508	2.5	1000	2.5	0.8	1	0	0	2.99	6	18	I
Phthalic anhydride	1.3	2000	0.7	1000	2	0	0	364	0.7	91	0.1	550	2.5	1000	1	0.4	1	2	2.66	1.46	4.5	18.6	
1,2-Dichloropropane	2.3	3000	0.4	5554	0.5	0	0	127	1.5	23	1.1	503	2.5	30	1.63	1.3	1.14	0	0.88	2.92	5.27	20	
Glycol ethers	0.8	1200	1	450	2.7	0	0	1490	0	373	0	9	1.25	1000	2.5	0	1	0	3.73	1.03	4.75	22.6	
Isobutyraldehyde	0.6	2810	0.4	6681	0.4	0	0	41	2.3	10	1.6	7	1.15	1000	2.5	-0.2	1	1	0.77	4.37	4.65	23.9	
Vinyl acetate	0.7	1613	0.8	3680	0.9	0	0	100	1.7	25	1	9	1.25	1000	2.5	-0.1	1	0	1.69	3.49	4.75	24.6	
Nitrobenzene	1.9	640	1.5	-99	0	0	0	119	1.5	30	0.9	9	1.23	1000	2.5	0.9	1	0	1.49	3.91	4.73	25.5	I
Toluene	2.7	5050	0	6675	0.4	0	0	34	2.4	4	2.3	10	1.27	1000	2.5	1.7	1.33	0	0.35	4.7	5.1	25.8	
Butyraldehyde	0.9	2490	0.5	7547	0.2	0	0	32	2.5	8	1.8	7	1.15	1000	2.5	0	1	1	0.75	4.82	4.65	25.9	
Diethanolamine	-1.4	710	1.4	484	2.6	0	0	4710	0	1178	0	9	1.25	1000	2.5	-2.1	1	0	4.04	1.41	4.75	25.9	
isopropyl alcohol	0.3	3600	0.2	32000	0	5	0	8623	0	2156	0	9	1.25	1000	2.5	-0.5	1	0	5.24	0.24	4.75	26	
Ethylene	1.1	9999	0	950000	0	0	0	14	3.1	3	2.4	10	1.28	1000	2.5	0.2	1	0	0	5.55	4.78	26.6	
Terephthalic acid	1.6	18800	0	-99	0	0	0	29	2.6	7	1.9	550	2.5	1000	2.5	0.7	1	0	0	4.45	6	26.7	I
Maleic anhydride	0.1	465	1.7	1000	2	3	0	2963	0	741	0	8	1.2	1000	1	-0.7	1	2	6.72	1.72	3.2	27	
1,4-Dioxane	-0.3	3150	0.3	6368	0.4	3.5	0	10352	0	2588	0	520	2.5	1000	2.5	-1	1	0	4.23	0.33	6	27.4	
Dimethyl phthalate	1.3	2400	0.5	500	2.6	0	0	121	1.5	30	0.9	9	1.25	400	2.43	0.4	1	0	3.13	2.93	4.68	28.4	
Hydroquinone	0.6	320	2	-99	0	0	0	141	1.4	35	0.8	9	1.25	1000	2.5	-0.2	1	0	1.99	4.17	4.75	29.3	I
Maneb	0	4400	0.1	-99	0	0	0	2	4.6	0.09	5	-99	1	-99	1	-99	1	0	0.09	9.67	3	29.3	Klbhc
1,1,1-Trichloroethane	2.5	11240	0	2000	1.4	0	0	48	2.2	7	1.9	503	2.5	30	1.63	1.5	1.24	0	1.4	4.11	5.37	29.5	
Pyridine	0.6	1580	0.8	1000	2	0	0	100	1.7	25	1	9	1.23	1000	2.5	-0.2	1	0	2.83	3.51	4.73	30	
Asbestos (friable)	0	9999	0	9999	0	5	0	-99	0	-99	0	9999	2.5	9999	2.5	1	1	0	5	0	6	30	KFN
Benzoyl chloride	2.2	2460	0.5	163	3.6	0	0	35	2.4	7	1.9	9	1.25	1000	1	1.2	1.12	2	4.09	4.89	3.37	30.3	
Propylene oxide	0	690	1.4	1740	1.5	4	0	306	0.9	77	0.2	9	1.25	1000	1	-0.8	1	2	6.95	2.48	3.25	30.7	
Dichloromethane	1.3	1600	0.8	17400	0	3.5	0	330	0.8	83	0.1	508	2.5	30	1.63	0.4	1	0	4.32	1.77	5.13	31.2	
Allyl chloride	-0.2	425	1.8	926	2.1	1.5	0	72	1.9	18	1.2	6	1.13	2	1	-1	1	0	5.35	4.92	3.13	32.1	
o-Xylene	2.8	5000	0	4550	0.7	0	0	16	3	2	2.8	10	1.27	1000	2.5	1.7	1.37	0	0.68	5.8	5.14	33.3	

HORIZONTAL TABLE: 10/6/93 ALGORITHM, 'OTHER SPECIFIC EFFECTS' EXCLUDED

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
Propylene	1.8	9999	0	10500	0	0	0	5	3.8	1	3.2	10	1.28	1000	2.5	0.8	1	0	0	6.97	4.78	33.4	
Carbaryl	2.4	500	1.7	25000	0	0	0	8	3.5	1	3.2	8	1.22	1000	1	1.4	1.18	2	1.67	8.35	3.4	34	
Diethyl phthalate	2.5	9000	0	537	2.5	0	0	32	2.5	5	2.2	9	1.25	400	2.43	1.5	1.23	0	2.54	4.68	4.91	35.5	
m-Xylene	3.2	5000	0	4550	0.7	0	0	16	3	2	3	10	1.27	1000	2.5	2.1	1.56	0	0.68	6.01	5.33	35.7	
Xylene (mixed isomers)	3	4300	0.1	6350	0.4	0	0	13	3.1	1	3.1	10	1.27	1000	2.5	1.9	1.47	0	0.5	6.3	5.24	35.7	
Butyl benzyl phthalate	4.8	2330	0.6	-99	0	0	0	43	2.3	2	2.7	8	1.2	400	2.43	3.5	2.26	0	0.55	5.56	5.69	36	I
Metolachlor	3.5	2780	0.4	-99	0	0	0	15	3	1	3.2	503	2.5	2	1	2.4	1.68	2	0.43	6.62	5.18	36.5	I
Manganese cmpds	0	615	1.5	-99	0	0	0	150	1.4	8	1.9	9999	2.5	9999	2.5	1	1	0	1.52	4.77	6	37.7	KI
Ethylbenzene	3.2	5460	0	5000	0.6	0	0	11	3.3	1	3.3	10	1.27	1000	2.5	2.1	1.54	0	0.6	6.59	5.31	38.2	
Chloroethane	1.4	7500	0	29	5	0	0	16	3	4	2.3	6	1.13	30	1.63	0.5	1	0	5	5.29	3.75	38.6	
Acrylic acid	0.4	193	2.4	1200	1.8	0	0	186	1.2	47	0.6	8	1.2	1000	2.5	-0.5	1	0	4.2	4.13	4.7	39.1	
Butylate	3.7	4659	0.1	-99	0	0	0	7	3.6	0.54	3.8	518	2.5	1000	1	2.5	1.77	2	0.05	7.43	5.27	39.4	I
Butyl acrylate	2.4	3730	0.2	2730	1.1	0	0	2	4.6	0.31	4.2	9	1.25	50	1.78	1.4	1.18	0	1.34	8.94	4.22	43.3	
Molybdenum trioxide	0	125	2.7	-99	0	0	0	370	0.7	19	1.2	9999	2.5	9999	2.5	-99	1	0	2.67	4.61	6	43.7	Klc
N,N-Dimethylaniline	2.3	1410	0.9	1225	1.8	0	0	65	2	12	1.6	513	2.5	1000	2.5	1.3	1.16	0	2.74	4.45	6.16	44.3	
Propionaldehyde	0.3	1200	1	4581	0.7	3	0	44	2.3	11	1.6	7	1.15	1000	2.5	-0.5	1	1	4.71	4.9	4.65	44.7	
Zinc compounds	0	7950	0	-99	0	0	0	17	2.9	0.86	3.4	9999	2.5	9999	2.5	3	2	0	0	6.39	7	44.7	KI
EPTC (ethyl dipropylthiocarbamate)	3.2	916	1.2	4062	0.8	0	0	27	2.6	3	2.6	9	1.25	1000	2.5	2.1	1.56	1	2.01	6.48	5.31	45.1	
Aniline	0.9	250	2.2	306	3	0	0	108	1.6	27	0.9	9	1.25	1000	2.5	0	1	0	5.2	4.73	4.75	47.2	
Bromomethane	1.2	214	2.3	780	2.2	0	0	11	3.3	3	2.6	6	1.13	30	1.63	0.3	1	0	4.5	8.15	3.75	47.4	
Chlorobenzene	2.8	1440	0.9	1100	1.9	0	0	17	3	2	2.8	6	1.13	1000	2.5	1.8	1.4	0	2.82	6.69	5.02	47.8	
Barium cmpds	0	132	2.6	-99	0	0	0	200	1.2	10	1.7	9999	2.5	9999	2.5	1	1	0	2.63	5.46	6	48.6	KI
Carbon tetrachloride	2.8	2800	0.4	19052	0	3.5	0	41	2.3	5	2.2	503	2.5	30	1.63	1.8	1.39	0	3.92	4.9	5.52	48.7	
Ethylene oxide	-0.3	270	2.1	835	2.2	4	0	474	0.5	118	0	510	2.5	12	1	-1.1	1	2	8.27	2.65	4.5	49.2	
Chloroform	2	908	1.2	5720	0.5	3.5	0	71	1.9	18	1.3	503	2.5	30	1.63	1	1	0	5.22	4.41	5.13	49.4	
Catechol	0.9	260	2.1	-99	0	0	0	9	3.4	2	2.7	9	1.25	1000	2.5	0	1	0	2.14	8.26	4.75	49.4	I
Alachlor	3.1	1065	1.1	-99	0	0	0	5	3.8	0.51	3.8	503	2.5	2	1	2	1.51	2	1.12	8.77	5.01	49.6	I
Benzene	2.1	4700	0	17500	0	5	0	19	2.9	4	2.3	10	1.27	1000	2.5	1.2	1.08	0	5.04	5.26	4.84	49.9	
Acetaldehyde	-0.2	1930	0.7	1500	1.6	3.5	0	34	2.4	9	1.8	7	1.15	1000	2.5	-1	1	1	5.84	4.92	4.65	50	
1,2-Dichloroethane	1.5	780	1.3	2063	1.4	3.5	0	136	1.4	34	0.8	508	2.5	30	1.63	0.6	1	0	6.22	3.57	5.13	50.2	
p-Xylene	3.2	5000	0	4550	0.7	0	0	2	4.5	0.2	4.5	10	1.27	1000	2.5	2.1	1.54	0	0.68	9	5.31	51.4	
Methylenebis(phenylisocyanate)	3.4	2200	0.6	5	5	0	0	66	2	6	2.1	550	2.5	1000	1	2.3	1.64	2	5.59	4.62	5.14	52.6	
1,2,4-Trimethylbenzene	3.4	5000	0	3655	0.9	0	0	8	3.5	0.68	3.6	502	2.5	1000	2.5	2.3	1.65	0	0.87	7.14	6.65	53.3	
Metam Sodium (MeNHCS2Na)	1	285	2.1	888	2.1	0	0	0.39	5	0.1	5	10	1.28	1	1	0.1	1	1	4.18	12.07	3.28	53.4	
Trichloroethylene	2.3	2402	0.5	8450	0.1	3.5	0	44	2.3	8	1.8	503	2.5	1000	2.5	1.3	1.15	0	4.18	4.62	6.15	54.1	
Toluene-2,4-diisocyanate	1.8	5800	0	10	5	3.5	0	53	2.1	13	1.5	550	2.5	1000	1	0.8	1	2	8.5	3.6	4.5	54.4	
Vinylidene chloride	1.8	200	2.3	6350	0.4	1.5	0	108	1.6	27	0.9	503	2.5	1000	2.5	0.9	1	0	4.22	4.89	6	54.7	
Chlorine dioxide	0	292	2.1	130	3.8	0	0	0.17	5	0.01	5	5	1.07	1	1	-99	1	0	5.83	12.06	3.07	54.9	Kc
Picric acid	2	30	3.7	-99	0	0	0	170	1.3	41	0.6	550	2.5	1000	2.5	1.1	1.03	0	3.7	5.63	6.03	56.3	I
Hydrochloric acid	1.1	900	1.2	277	3.1	0	0	19	2.9	0.95	3.4	10	1.28	1000	2.5	0.5	1	1	4.36	7.48	4.78	56.6	
Acrylonitrile	-0.9	78	3	576	2.5	4	0	10	3.3	3	2.7	5	1.07	1	1	-1.6	1	0	9.49	9	3.07	56.8	
Cumene hydroperoxide	2.3	382	1.9	200	3.4	1	0	62	2	11	1.6	9	1.23	1000	2.5	1.3	1.14	0	6.26	5.45	4.87	57	
1,4-Dichlorobenzene	3.4	3790	0.2	1100	1.9	3.5	0	34	2.5	3	2.5	6	1.13	1000	2.5	2.3	1.65	0	5.62	5.2	5.27	57.1	
Cyanazine	1.9	261	2.1	230	3.3	0	0	18	2.9	5	2.2	503	2.5	1	1	0.9	1	2	5.41	7.29	4.5	57.2	
Cumene	3.7	2910	0.4	8000	0.2	0	0	6	3.7	0.49	3.8	502	2.5	1000	2.5	2.5	1.77	0	0.59	7.9	6.77	57.5	
Phenol	1.5	530	1.6	46	4.7	0	0	34	2.4	8	1.8	9	1.25	1000	2.5	0.6	1	0	6.3	5.86	4.75	57.8	
Atrazine	2.3	1750	0.8	540	2.5	0	0	16	3	3	2.6	503	2.5	1000	2.5	1.3	1.17	0	3.3	6.35	6.17	59.5	
Phosphorus (yellow or white)	3	3	5	-99	0	0	0	0.02	5	0	5	-99	1	0	1	1	1	0	5	15	3	60	lb
Chloroprene	1.4	260	2.1	3253	1	0	0	2	4.4	0.56	3.8	503	2.5	2	1	0.5	1	0	3.12	10.32	4.5	60.5	
Captan	1.8	7500	0	168	3.5	0	0	0.2	5	0.05	5	503	2.5	30	1	0.9	1	2	3.55	10	4.5	61	

HORIZONTAL TABLE: 10/6/93 ALGORITHM, 'OTHER SPECIFIC EFFECTS' EXCLUDED

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
Di-n-octyl phthalate	5.2	13000	0	-99	0	0	0	0.93	5	0.05	5	9	1.23	400	2.43	3.9	2.44	0	0	10	6.1	61	I
Tetrachloroethylene	2.6	8100	0	5200	0.6	3.5	0	17	3	2	2.7	503	2.5	1000	2.5	1.6	1.29	0	4.07	5.67	6.29	61.2	
Cresol (mixed isomers)	2	760	1.4	50	4.6	0	0	13	3.2	3	2.5	9	1.23	1000	2.5	1	1	0	5.97	7.01	4.73	61.4	
Bis(2-ethylhexyl) adipate	5.9	9110	0	-99	0	0	0	0.35	5	0.02	5	9	1.25	1000	2.5	4.2	2.5	0	0	10	6.25	62.5	I
Hexachloroethane	3.3	4970	0	10000	0	1.5	0	1	4.8	0.13	4.8	503	2.5	30	1.63	2.2	1.59	0	1.5	9.56	5.71	63.2	
Acrylamide	-0.7	107	2.8	1000	2	3.5	0	109	1.6	27	0.9	9	1.25	360	2.4	-1.4	1	0	8.28	5.33	4.65	63.3	
Chlorophenols [o]	2.3	261	2.1	100	4	0	0	19	2.9	3	2.4	6	1.13	1000	2.5	1.3	1.15	0	6.14	7.45	4.78	64.9	
4,4'-Isopropylidenediphenol	3.3	2500	0.5	200	3.4	0	0	5	3.9	0.42	4	8	1.2	1000	2.5	2.2	1.62	0	3.9	8.36	5.31	65.1	
p-Cresol	2	207	2.3	50	4.6	0	0	25	2.7	6	2	9	1.23	1000	2.5	1	1	0	6.91	6.98	4.73	65.8	
Malathion	2.9	570	1.6	6	5	0	0	0.1	5	0.01	5	9	1.25	1000	1	1.8	1.4	2	6.57	11.57	3.66	66.3	
Phosphoric acid	-0.6	1530	0.9	14	5	0	0	70	1.9	4	2.4	9999	2.5	1000	2.5	-0.9	1	1	5.86	5.21	6	66.4	
Vinyl chloride	1.5	500	1.7	100	4	5	0	143	1.4	36	0.7	6	1.13	1000	2.5	0.6	1	0	10.67	3.82	4.63	67	
Chlorine	0	8910	0	34	4.9	0	0	0.34	5	0.02	5	9999	2.5	1	1	1	1	0	4.93	10	4.5	67.2	K
Dichlorobenzene (mixed isomers)	3.4	2600	0.5	1100	1.9	0	0	0.54	5	0.05	5	6	1.13	1000	2.5	2.3	1.65	0	2.39	10.47	5.27	67.9	
1,3-butadiene	2	3210	0.3	128850	0	3.5	0	4	4	1	3.3	502	2.5	1000	2.5	1	1.01	0	3.82	7.62	6.01	68.8	
4-nitrophenol	0.8	620	1.5	50	4.6	0	0	41	2.3	10	1.6	550	2.5	1000	2.5	-0.1	1	0	6.11	5.47	6	69.5	
Ammonia	-0.8	350	1.9	2377	1.2	0	0	2	4.6	0.09	5	9	1.25	1000	2.5	-1.2	1	1	3.17	11.5	4.75	69.7	
Cyclohexane	3.4	29820	0	500	2.6	0	0	5	3.9	0.39	4	502	2.5	1000	2.5	2.3	1.67	0	2.6	7.92	6.67	70.2	
1,2-Dichlorobenzene	3.4	1400	0.9	1700	1.5	0	0	0.55	5	0.05	5	6	1.13	1000	2.5	2.3	1.64	0	2.46	10.92	5.27	70.5	
Sulfuric acid	-1.1	2140	0.6	14	5	0	0	31	2.5	2	3	9999	2.5	1000	2.5	-1.3	1	1	5.61	6.14	6	70.6	
Methyl Parathion	3.2	14	4.3	3	5	0	0	9	3.4	0.88	3.4	0	1	1000	1	2.1	1.54	2	9.25	11.1	3.54	72	
4,4'-Methylenedianiline	1.6	185	2.4	163	3.6	3.5	0	45	2.2	11	1.6	8	1.22	1000	2.5	0.7	1	0	9.46	6.2	4.72	73.9	
2,4-Dinitrotoluene	2	268	2.1	-99	0	3.5	0	24	2.7	6	2	550	2.5	1000	2.5	1	1.01	0	5.62	6.84	6.01	74.8	I
Dibutyl phthalate	4.9	9000	0	500	2.6	0	0	1	5	0.05	5	9	1.23	400	2.43	3.6	2.31	0	2.6	9.98	5.98	75.2	
1,1,2-Trichloroethane	2.2	150	2.5	2000	1.4	1.5	0	7	3.6	1	3.1	503	2.5	30	1.63	1.2	1.09	0	5.44	9.24	5.22	76.6	
Naphthalene	3.2	2200	0.6	30	5	1	0	6	3.7	0.59	3.7	9	1.23	1000	2.5	2.1	1.56	0	6.59	7.99	5.3	77.3	
N-nitrosodiphenylamine	3.1	1650	0.8	-99	0	3.5	0	1	4.8	0.13	4.8	8	1.22	1000	2.5	2.1	1.53	1	4.3	10.45	5.25	77.4	I
Styrene	3	1000	1.2	2528	1.2	3.5	0	4	4	0.44	3.9	10	1.27	1000	2.5	1.9	1.45	0	5.86	9.08	5.22	77.9	
2,4-D	3.5	275	2.1	-99	0	3.5	0	71	1.9	6	2.1	503	2.5	1000	2.5	2.4	1.71	0	5.6	6.07	6.71	78.4	I
Epichlorohydrin	0.3	40	3.5	500	2.6	3.8	0	35	2.4	9	1.8	510	2.5	30	1	-0.5	1	2	9.85	7.68	4.5	78.9	
Di(2-ethylhexyl) phthalate	4.9	30000	0	-99	0	3.5	0	1	4.7	0.08	5	9	1.23	400	2.43	3.6	2.31	0	3.5	9.72	5.97	79	I
Titanium tetrachloride	0	1000	1.2	7	5	0	0	25	2.7	1	3.2	9999	2.5	9999	2.5	-99	1	1	6.17	7.01	6	79	Kc
Hydrogen fluoride	0	50	3.3	86	4.1	0	0	265	1	13	1.5	9999	2.5	1000	2.5	-0.4	1	0	7.47	5.76	6	79.4	
2,4-Dinitrophenol	1.5	30	3.7	-99	0	0	0	11	3.3	3	2.6	550	2.5	1000	2.5	0.6	1	0	3.7	9.56	6	79.6	I
Nitric acid	0.2	500	1.7	65	4.4	0	0	26	2.6	1	3.1	9999	2.5	1000	2.5	-0.3	1	1	6.04	7.45	6	81	
Decabromodiphenyl oxide	5.2	2570	0.5	-99	0	0	0	0.06	5	0	5	550	2.5	1000	2.5	3.9	2.44	0	0.48	10.48	7.44	81.6	I
Chlorpyrifos	5	151	2.5	-99	0	0	0	2	4.4	0.12	4.9	503	2.5	1000	1	3.7	2.35	2	2.53	11.77	5.85	83.7	I
Copper cmpds	0	300	2	-99	0	0	0	0.33	5	0.02	5	9999	2.5	9999	2.5	-1	1	0	2.04	12.04	6	84.4	KI
Biphenyl	4	3280	0.3	25	5	0	0	2	4.6	0.12	4.9	9	1.23	1000	2.5	2.8	1.9	0	5.31	9.82	5.64	85.2	
Lead cmpds	0	1500	0.9	-99	0	3.5	0	5	3.8	0.26	4.3	9999	2.5	9999	2.5	1.8	1.39	0	4.37	9.01	6.39	85.5	KI
Chlorothalonil	5	6000	0	7	5	0	0	0.05	5	0	5	550	2.5	1	1	3.7	2.36	0	5	10	5.86	87.9	
Hexachlorobenzene	4.1	4000	0.2	308	3	3.5	0	22	2.8	1	3.1	550	2.5	1000	2.5	3	1.98	0	6.68	5.99	6.98	88.5	
Hydrogen cyanide	0	4	5	18	5	0	0	1385	0	346	0	9999	2.5	1000	2.5	-0.7	1	0	10	5	6	90	
Nickel cmpds	0	350	1.9	-99	0	5	0	27	2.6	1	3.1	9999	2.5	9999	2.5	1.6	1.3	0	6.93	7.68	6.3	92	KI
1,3-dichloropropene	2	140	2.6	996	2	3.5	0	0.24	5	0.06	5	508	2.5	2	1	1	1	1	8.09	12.59	4.5	93.1	
Formaldehyde	1.1	260	2.1	480	2.6	4	0	24	2.7	6	2	502	2.5	1000	2.5	0.2	1	0	8.78	6.87	6	93.9	
2-nitropropane	1.1	725	1.4	600	2.4	3.5	0	5	3.9	1	3.2	550	2.5	1000	2.5	0.2	1	0	7.34	8.49	6	95	
Diaminotoluene (mixed isomers) [24]	1.4	260	2.1	100	4	3.5	0	37	2.4	9	1.7	550	2.5	1000	2.5	0.5	1	0	9.64	6.25	6	95.4	
Anthracene	4.5	17000	0	250	3.2	1	0	0.01	5	0	5	502	2.5	1000	2.5	3.2	2.12	0	4.2	10	7.12	101.2	
Trifluralin	3.1	500	1.7	47	4.7	0	0	0.11	5	0.01	5	503	2.5	30	1.63	2	1.5	0	6.33	11.67	5.62	101.2	

HORIZONTAL TABLE: 10/6/93 ALGORITHM, 'OTHER SPECIFIC EFFECTS' EXCLUDED

chemical	log Kow	oral (mg/kg)	HV	inhal (ppm)	HV	ncar	ntox	fish (mg/l)	HV	noeff (mg/l)	HV	BOD (days)	HV	hydr (days)	HV	logbcf	HV	water react	heal	envi	mult	sum	bad (a)
1,2,4-Trichlorobenzene	4	300	2	1100	1.9	0	0	3	4.2	0.2	4.5	550	2.5	1000	2.5	2.9	1.93	0	3.95	10.73	6.93	101.8	
Cobalt cmpds	0	55	3.3	-99	0	0	0	0.38	5	0.02	5	9999	2.5	9999	2.5	1.7	1.35	0	3.26	13.26	6.35	105	KI
Chromium cmpds	0	97	2.9	-99	0	5	0	33	2.5	2	3	9999	2.5	9999	2.5	2.3	1.65	0	7.85	8.29	6.65	107.3	KI
Polychlorinated biphenyls	6.3	1300	1	-99	0	3.8	0	3	4.3	0.14	4.8	550	2.5	1000	2.5	4.2	2.5	0	4.73	10.02	7.5	110.6	I
Hexachloro-1,3-butadiene	4.9	102	2.8	35	4.9	1.5	0	0.09	5	0	5	503	2.5	2	1	3.6	2.31	0	9.23	12.82	5.81	128.2	
Arsenic cmpds	0	8	4.7	-99	0	5	0	32	2.5	2	3	9999	2.5	9999	2.5	2.5	1.75	1	9.66	10.14	6.75	133.7	KI
Terbufos (tBuSCH2SP(=S)(OEt)2	4.5	3	5	1	5	0	0	0.01	5	0	5	508	2.5	15	1.41	3.3	2.15	1	10	15	6.06	151.6	
Cadmium cmpds	0	88	2.9	306	3	4	0	0.1	5	0	5	9999	2.5	9999	2.5	3.5	2.25	0	9.95	12.92	7.25	165.9	K

(a): Missing/no QSAR: I=inhl, O=oral, N=Fish Noefft, F=Fish, K=logKow, b=BOD, h=Hydro, c=log BCF

APPENDIX D
RANKING RESULTS: CHEMICAL SCORES

TOTAL HAZARD VALUES AND CHEMICAL RANKS, WEIGHTED BY RELEASES

chemical	Hazard Value (normalized)		Chemical Rank	
	default=0	default=5	default=0	default=5
Chromium cmpds	100	100	1	1
Arsenic cmpds	98.7	91.9	2	3
Lead cmpds	95.3	95.7	3	2
Copper cmpds	86.7	90	4	4
Terbufos (tBuSCH2SP(=S)(OEt)2	85.3	72.9	5	7
2,4-D	84.6	75.5	6	6
Nickel cmpds	84.4	83.8	7	5
Formaldehyde	83.7	71.6	8	8
1,3-dichloropropene	77.5	66.3	9	9
Trifluralin	76.1	65.1	10	10
Cadmium cmpds	74.9	64	11	11
Ammonia	72.5	62	12	13
Sulfuric acid	72.1	61.6	13	14
Hydrogen fluoride	67.2	57.5	14	16
Nitric acid	64.5	55.1	15	18
Hydrochloric acid	63.9	54.6	16	19
Styrene	62.2	53.2	17	23
Chlorpyrifos	60.3	54.3	18	21
Hydrogen cyanide	58.4	49.9	19	25
Tetrachloroethylene	58.3	49.8	20	26
Trichloroethylene	56.1	48	21	29
Chlorine	55.6	47.5	22	30
Manganese cmpds	54.1	61.3	23	15
Chlorothalonil	53.9	46.1	24	32
Di(2-ethylhexyl) phthalate	52.7	56.1	25	17
Hexachlorobenzene	49.9	42.7	26	35
Naphthalene	48.4	41.4	27	36
Phosphoric acid	48.3	41.3	28	37
Cobalt cmpds	48.2	46.3	29	31
Phenol	47.1	40.3	30	38
Barium cmpds	46.6	50.4	31	24
Polychlorinated biphenyls	46	42.9	32	34
Benzene	44.6	38.1	33	40
Captan	44.3	37.9	34	41
Acrylamide	43.9	37.5	35	42
Alachlor	43.6	39.7	36	39
Chloroform	43.2	37	37	43
Biphenyl	43.2	36.9	38	44
Acrylonitrile	42.5	36.3	39	47
1,2,4-Trichlorobenzene	42.3	36.1	40	48
1,2-Dichloroethane	42.1	36	41	49
Zinc compounds	41.7	53.3	42	22
Xylene (mixed isomers)	41.3	35.3	43	50
Atrazine	41.1	35.2	44	51
1,3-butadiene	39.4	33.7	45	52
Decabromodiphenyl oxide	38.4	36.3	46	46
2,4-Dinitrotoluene	38.2	36.5	47	45
1,1,1-Trichloroethane	38.1	32.6	48	53
Methyl Parathion	36.9	31.6	49	54
Metam Sodium (MeNHCS2Na)	36.9	31.5	50	55
Phosphorus (yellow or white)	36.7	49.2	51	27
Malathion	35.7	30.5	52	57
Ethylene oxide	34.9	29.8	53	58

TOTAL HAZARD VALUES AND CHEMICAL RANKS, WEIGHTED BY RELEASES

chemical	Hazard Value (normalized)		Chemical Rank	
	default=0	default=5	default=0	default=5
Cyanazine	34.6	29.6	54	59
Carbaryl	33.3	28.5	55	61
Dibutyl phthalate	33.1	28.3	56	62
2,4-Dinitrophenol	33	31	57	56
Carbon disulfide	32.7	28	58	63
2-nitropropane	32.6	27.9	59	64
EPTC (ethyldipropylthiocarbamate)	32.3	27.6	60	65
Cyclohexane	32.1	27.4	61	66
Cresol (mixed isomers)	31.8	27.2	62	67
Metolachlor	31.7	29.5	63	60
Dichloromethane	31.1	26.6	64	68
Ethylbenzene	30.7	26.3	65	69
Epichlorohydrin	30.5	26	66	70
Toluene	30.4	26	67	71
Vinyl chloride	29.8	25.5	68	73
Acetaldehyde	29.7	25.4	69	74
Acrylic acid	28.9	24.7	70	75
Diaminotoluene (mixed isomers)[24]	28.6	24.4	71	77
p-Cresol	28.4	24.3	72	79
Aniline	27.9	23.8	73	81
Anthracene	27.3	23.4	74	83
Maneb	26.9	48.8	75	28
Carbon tetrachloride	26.7	22.9	76	84
Chloroprene	26.5	22.6	77	85
Butylate	25.4	24.2	78	80
Picric acid	25.2	24.4	79	78
Molybdenum trioxide	25	25.7	80	72
Chlorobenzene	24.8	21.2	81	87
Cumene	24.4	20.9	82	88
1,2,4-Trimethylbenzene	24.3	20.7	83	89
Asbestos (friable)	23.9	54.4	84	20
1,2-Dichlorobenzene	23.3	19.9	85	91
4-nitrophenol	23	19.7	86	92
Propylene oxide	22.3	19	87	93
Zinc (fume or dust)	22.3	63	88	12
Methyl ethyl ketone	22.1	18.9	89	94
Isopropyl alcohol	21.8	18.6	90	95
Methylenebis(phenylisocyanate)	21.2	18.1	91	97
4,4'-Isopropylidenediphenol	20.8	17.7	92	99
Bis(2-ethylhexyl) adipate	19.8	20.1	93	90
1,4-Dichlorobenzene	19.2	16.4	94	100
o-Xylene	19.1	16.3	95	101
Catechol	19.1	18.6	96	96
4,4'-Methylenedianiline	18.6	15.9	97	103
Glycol ethers	17.7	15.2	98	104
Terephthalic acid	17.7	24.7	99	76
1,1,2-Trichloroethane	17.6	15	100	105
Cumene hydroperoxide	17	14.5	101	108
Butyl benzyl phthalate	16.7	21.3	102	86
Hexachloro-1,3-butadiene	16.1	13.7	103	110
Chlorine dioxide	16.1	13.7	104	111
Chloromethane	15.9	13.6	105	112
2-methoxyethanol	15.4	13.2	106	114

TOTAL HAZARD VALUES AND CHEMICAL RANKS, WEIGHTED BY RELEASES

chemical	Hazard Value (normalized)		Chemical Rank	
	default=0	default=5	default=0	default=5
Vinyl acetate	15.2	13	107	115
p-Xylene	15	12.9	108	116
m-Xylene	14.8	12.6	109	117
Hydroquinone	14.7	14.8	110	106
N,N-Dimethylaniline	14.6	12.5	111	118
Methyl isobutyl ketone	14	11.9	112	120
Chloroethane	13.9	11.9	113	121
n-butyl alcohol	13.5	11.6	114	122
Bromomethane	13.1	11.2	115	123
Metribuzin	12.9	13.9	116	109
Nitrobenzene	12.8	13.2	117	113
Phthalic anhydride	12.6	10.8	118	124
Pyridine	12.6	10.7	119	125
Vinylidene chloride	12.4	10.6	120	126
Maleic anhydride	12.3	10.5	121	127
2-ethoxyethanol	12.2	10.4	122	128
Propionaldehyde	12.1	10.3	123	129
Titanium tetrachloride	11.9	10.2	124	131
1,4-Dioxane	11.8	10.1	125	132
Diethanolamine	11.7	10	126	133
Chlorophenols [o]	11.7	10	127	134
Methyl methacrylate	11.1	9.5	128	135
Ethylene glycol	10.8	9.2	129	136
Ammonium nitrate (solution)	10.6	23.4	130	82
Toluene-2,4-diisocyanate	10.5	9	131	137
Di-n-octyl phthalate	10.2	17.8	132	98
Antimony cmpds	10.1	16	133	102
Butyraldehyde	9.7	8.3	134	139
Dichlorobenzene (mixed isomers)	9.7	8.3	135	138
N-nitrosodiphenylamine	9.1	10.3	136	130
Dimethyl phthalate	8.9	7.6	137	140
Hexachloroethane	8.9	7.6	138	141
Diethyl phthalate	8.7	7.4	139	142
Aluminum (fume or dust)	8.4	45.2	140	33
Acetonitrile	7.9	6.7	141	143
Freon 113	7.6	6.5	142	144
Acetone	7.5	6.4	143	145
Benzoyl chloride	7.2	6.1	144	146
Allyl chloride	7.1	6.1	145	147
Ethylene	6.9	5.9	146	148
Butyl acrylate	5.6	4.8	147	149
Methanol	5.1	4.4	148	150
Ammonium sulfate (solution)	5.1	14.7	149	107
Isobutyraldehyde	4.9	4.1	150	151
Carbonyl sulfide	4.4	3.8	151	152
Propylene	3.7	3.2	152	154
1,2-Dichloropropane	3.1	2.7	153	155
tert-butyl alcohol	2.2	1.9	154	156
Thorium dioxide	2	12.4	155	119
Glyphosate	1.4	3.5	156	153
Methyl tert-butyl ether	0.6	0.5	157	157
sec-butyl alcohol	0.4	0.3	158	158

TOTAL HAZARD VALUES AND CHEMICAL RANKS, WEIGHTED BY RELEASES

chemical	Hazard Value (normalized)		Chemical Rank	
	'other specific effects' used	'other specific effects' excl.	'other specific effects' used	'other specific effects' excl.
Chromium cmpds	100	100	1	1
Arsenic cmpds	98.7	91	2	2
Lead cmpds	95.3	77.9	3	6
Copper cmpds	86.7	80.5	4	4
Terbufos (tBuSCH2SP(=S)(OEt)2	85.3	90.6	5	3
2,4-D	84.6	71.4	6	10
Nickel cmpds	84.4	74.3	7	7
Formaldehyde	83.7	73.8	8	8
1,3-dichloropropene	77.5	78.2	9	5
Trifluralin	76.1	66.5	10	14
Cadmium cmpds	74.9	69.5	11	12
Ammonia	72.5	71.6	12	9
Sulfuric acid	72.1	69.8	13	11
Hydrogen fluoride	67.2	53	14	19
Nitric acid	64.5	68.5	15	13
Hydrochloric acid	63.9	62.2	16	16
Styrene	62.2	52.5	17	20
Chlorpyrifos	60.3	64	18	15
Hydrogen cyanide	58.4	57.6	19	17
Tetrachloroethylene	58.3	40.8	20	30
Trichloroethylene	56.1	37.5	21	41
Chlorine	55.6	54.4	22	18
Manganese cmpds	54.1	38.9	23	36
Chlorothalonil	53.9	48.3	24	22
Di(2-ethylhexyl) phthalate	52.7	42.3	25	29
Hexachlorobenzene	49.9	38.2	26	38
Naphthalene	48.4	44.5	27	25
Phosphoric acid	48.3	51.3	28	21
Cobalt cmpds	48.2	48.2	29	23
Phenol	47.1	42.3	30	28
Barium cmpds	46.6	39.7	31	33
Polychlorinated biphenyls	46	40.6	32	31
Benzene	44.6	35.2	33	44
Captan	44.3	34.2	34	48
Acrylamide	43.9	34.9	35	45
Alachlor	43.6	46.3	36	24
Chloroform	43.2	33.1	37	51
Biphenyl	43.2	39.7	38	32
Acrylonitrile	42.5	38.4	39	37
1,2,4-Trichlorobenzene	42.3	37.9	40	39
1,2-Dichloroethane	42.1	30.9	41	55
Zinc compounds	41.7	44.3	42	26
Xylene (mixed isomers)	41.3	27.4	43	61
Atrazine	41.1	43.7	44	27
1,3-butadiene	39.4	26.2	45	68
Decabromodiphenyl oxide	38.4	34.4	46	46
2,4-Dinitrotoluene	38.2	32.6	47	52
1,1,1-Trichloroethane	38.1	23.5	48	73
Methyl Parathion	36.9	39.2	49	34
Metam Sodium (MeNHCS2Na)	36.9	39.1	50	35
Phosphorus (yellow or white)	36.7	35.4	51	43
Malathion	35.7	37.9	52	40
Ethylene oxide	34.9	23.7	53	72

TOTAL HAZARD VALUES AND CHEMICAL RANKS, WEIGHTED BY RELEASES

chemical	Hazard Value (normalized)		Chemical Rank	
	'other specific effects' used	'other specific effects' excl.	'other specific effects' used	'other specific effects' excl.
Cyanazine	34.6	36.7	54	42
Carbaryl	33.3	25.3	55	70
Dibutyl phthalate	33.1	27.5	56	60
2,4-Dinitrophenol	33	28.5	57	57
Carbon disulfide	32.7	11.1	58	113
2-nitropropane	32.6	28.2	59	58
EPTC (ethyldipropylthiocarbamate)	32.3	34.3	60	47
Cyclohexane	32.1	34.1	61	49
Cresol (mixed isomers)	31.8	31	62	54
Metolachlor	31.7	33.6	63	50
Dichloromethane	31.1	27.9	64	59
Ethylbenzene	30.7	21.1	65	79
Epichlorohydrin	30.5	25	66	71
Toluene	30.4	21	67	80
Vinyl chloride	29.8	22.8	68	74
Acetaldehyde	29.7	31.5	69	53
Acrylic acid	28.9	26.9	70	63
Diaminotoluene (mixed isomers)[24]	28.6	26.3	71	67
p-Cresol	28.4	30.1	72	56
Aniline	27.9	26.5	73	66
Anthracene	27.3	26.7	74	65
Maneb	26.9	20.2	75	83
Carbon tetrachloride	26.7	18.5	76	88
Chloroprene	26.5	17.5	77	92
Butylate	25.4	26.9	78	62
Picric acid	25.2	26.8	79	64
Molybdenum trioxide	25	20.8	80	81
Chlorobenzene	24.8	20	81	84
Cumene	24.4	17.4	82	93
1,2,4-Trimethylbenzene	24.3	25.8	83	69
Asbestos (friable)	23.9	21.1	84	78
1,2-Dichlorobenzene	23.3	22.6	85	75
4-nitrophenol	23	19.7	86	85
Propylene oxide	22.3	14.7	87	100
Zinc (fume or dust)	22.3	7.1	88	133
Methyl ethyl ketone	22.1	4.4	89	142
Isopropyl alcohol	21.8	16.8	90	94
Methylenebis(phenylisocyanate)	21.2	22.5	91	76
4,4'-Isopropylidenediphenol	20.8	22	92	77
Bis(2-ethylhexyl) adipate	19.8	19	93	86
1,4-Dichlorobenzene	19.2	17.7	94	91
o-Xylene	19.1	12	95	109
Catechol	19.1	20.3	96	82
4,4'-Methylenedianiline	18.6	18.3	97	89
Glycol ethers	17.7	18.8	98	87
Terephthalic acid	17.7	15.3	99	96
1,1,2-Trichloroethane	17.6	16.4	100	95
Cumene hydroperoxide	17	18	101	90
Butyl benzyl phthalate	16.7	15.1	102	97
Hexachloro-1,3-butadiene	16.1	15	103	98
Chlorine dioxide	16.1	12.9	104	104
Chloromethane	15.9	9	105	125
2-methoxyethanol	15.4	7.9	106	131

TOTAL HAZARD VALUES AND CHEMICAL RANKS, WEIGHTED BY RELEASES

chemical	Hazard Value (normalized)		Chemical Rank	
	'other specific effects' used	'other specific effects' excl.	'other specific effects' used	'other specific effects' excl.
Vinyl acetate	15.2	12.9	107	103
p-Xylene	15	9.3	108	122
m-Xylene	14.8	10.5	109	115
Hydroquinone	14.7	13.4	110	102
N,N-Dimethylaniline	14.6	11.5	111	111
Methyl isobutyl ketone	14	6.8	112	135
Chloroethane	13.9	14.7	113	99
n-butyl alcohol	13.5	10.1	114	118
Bromomethane	13.1	9.7	115	120
Metribuzin	12.9	13.7	116	101
Nitrobenzene	12.8	9.9	117	119
Phthalic anhydride	12.6	8.5	118	128
Pyridine	12.6	11.2	119	112
Vinylidene chloride	12.4	8.2	120	130
Maleic anhydride	12.3	11.5	121	110
2-ethoxyethanol	12.2	5.3	122	140
Proplonaldehyde	12.1	10.8	123	114
Titanium tetrachloride	11.9	12.6	124	105
1,4-Dioxane	11.8	12.5	125	106
Diethanolamine	11.7	12.5	126	107
Chlorophenols [o]	11.7	12.4	127	108
Methyl methacrylate	11.1	3.2	128	147
Ethylene glycol	10.8	7.1	129	134
Ammonium nitrate (solution)	10.6	5.5	130	138
Toluene-2,4-diisocyanate	10.5	10.1	131	117
Di-n-octyl phthalate	10.2	8.5	132	129
Antimony cmpds	10.1	3	133	149
Butyraldehyde	9.7	10.3	134	116
Dichlorobenzene (mixed isomers)	9.7	9	135	126
N-nitrosodiphenylamine	9.1	9.1	136	124
Dimethyl phthalate	8.9	9.5	137	121
Hexachloroethane	8.9	7.4	138	132
Diethyl phthalate	8.7	9.2	139	123
Aluminum (fume or dust)	8.4	8.9	140	127
Acetonitrile	7.9	1	141	154
Freon 113	7.6	3.3	142	146
Acetone	7.5	2.9	143	150
Benzoyl chloride	7.2	5.8	144	137
Allyl chloride	7.1	5.2	145	141
Ethylene	6.9	3.1	146	148
Butyl acrylate	5.6	6	147	136
Methanol	5.1	0	148	158
Ammonium sulfate (solution)	5.1	5.4	149	139
Isobutyraldehyde	4.9	3.3	150	144
Carbonyl sulfide	4.4	0	151	157
Propylene	3.7	3.9	152	143
1,2-Dichloropropane	3.1	3.3	153	145
tert-butyl alcohol	2.2	2.3	154	151
Thorium dioxide	2	2.1	155	152
Glyphosate	1.4	1.5	156	153
Methyl tert-butyl ether	0.6	0.7	157	155
sec-butyl alcohol	0.4	0.4	158	158

TOTAL HAZARD VALUES AND CHEMICAL RANKS, NOT WEIGHTED BY RELEASES

Chemical	Hazard value				Chemical rank			
	Even weight	Double carcin. weight	Half human acute	Half environ. weight	Even weight	Double carcin. weight	Half human acute	Half environ. weight
Cadmium compounds	100	100	100	100	1	1	1	1
Arsenic compounds	82	86.6	83.2	85	2	2	2	2
Terbufos (tBuSCH2SP(=S)(OEt)2	80.8	70	73.1	75.4	3	5	5	4
Hexachloro-1,3-butadiene	77.6	71.3	74.2	77	4	4	4	3
Polychlorinated biphenyls	70.9	74.4	78	67.9	5	3	3	6
Trifluralin	62.9	54.5	60.4	60.6	6	15	14	13
Hexachlorobenzene	62.1	65	63.5	67.9	7	8	7	5
1,2,4-Trichlorobenzene	61.7	53.4	61.4	55.8	8	16	11	17
Chromium compounds	60.8	68	62.9	61.4	9	6	9	11
2-nitropropane	60.2	61.9	61.1	62.2	10	10	12	9
Formaldehyde	59.6	62.7	58.8	64.9	11	9	15	7
Cobalt compounds	59.3	51.4	60.8	49.2	12	23	13	28
Lead compounds	59.2	61.6	65.2	58.5	13	11	6	14
Nickel compounds	59.1	65.8	63.2	61.6	14	7	8	10
Anthracene	57.7	53.3	58.4	51.6	15	17	16	21
Diaminotoluene (mixed isomers)[2	57.2	59.3	53.6	62.9	16	12	21	8
Hydrogen fluoride	55.1	47.7	48.8	61.2	17	26	31	12
Di(2-ethylhexyl) phthalate	54.8	57.2	62	52.5	18	13	10	20
Chlorothalonil	53.1	46	51.2	50	19	29	27	23
2,4-D	52.5	56.3	55.1	55.5	20	14	19	18
2,4-Dinitrophenol	52	52.4	52.6	49.2	21	21	23	27
1,3-dichloropropene	52	45	52.1	48.9	22	31	25	29
Epichlorohydrin	51.6	52.5	50.1	56.6	23	20	29	16
Decabromodiphenyl oxide	51.4	44.6	57	40.8	24	33	17	46
Biphenyl	51.4	44.6	49.1	48.9	25	32	30	30
Copper compounds	51.4	44.5	54.4	42.9	26	34	20	39
Hydrogen cyanide	51.2	44.3	39.8	57.6	27	35	48	15
Styrene	49.9	51.6	52.7	49.7	28	22	22	24
Dibutyl phthalate	49.6	43	51.4	45	29	38	26	37
2,4-Dinitrotoluene	49.5	52.6	52.1	51.4	30	18	24	22
1,3-butadiene	49.5	52.6	55.3	49.7	31	19	18	25
Naphthalene	46.8	43	44	47.4	32	37	37	32

TOTAL HAZARD VALUES AND CHEMICAL RANKS, NOT WEIGHTED BY RELEASES

Chemical	Hazard value				Chemical rank			
	Even weight	Double carcin. weight	Half human acute	Half environ. weight	Even weight	Double carcin. weight	Half human acute	Half environ. weight
Tetrachloroethylene	46	50.1	51	48.7	33	25	28	31
Vinyl chloride	45.6	50.2	43.6	54.5	34	24	38	19
Chlorpyrifos	44.6	38.7	46	35	35	45	35	59
Chloroprene	44.2	38.3	45.7	42.4	36	46	36	40
N-nitrosodiphenylamine	44.1	46.6	48.5	39.2	37	27	32	48
Acrylamide	43.6	45.3	42.6	49.4	38	30	41	26
1,1,2-Trichloroethane	43.6	41.4	43.1	41	39	40	39	45
4-nitrophenol	43.4	37.6	38.1	46.2	40	49	54	34
Nitric acid	43.2	37.4	37.8	41.6	41	50	55	41
Hexachloroethane	42.8	41	48.4	37.7	42	41	33	51
Titanium tetrachloride	42.1	36.5	36.5	41.2	43	52	59	44
Captan	42.1	36.5	42.8	40.1	44	53	40	47
Trichloroethylene	41.9	46.3	46.2	45.8	45	28	34	35
4,4'-Methylenedianiline	41.9	43.9	38.9	45.4	46	36	49	36
Sulfuric acid	40.8	35.3	36	41.3	47	55	62	42
1,2-Dichlorobenzene	40.4	35	41.8	33.4	48	56	42	65
Ammonia	39.7	34.4	40.3	33.5	49	58	46	63
Dichlorobenzene (mixed isomers)	39	33.8	40.3	32.3	50	59	47	66
Vinylidene chloride	38.7	37.7	38.9	41.2	51	48	50	43
Methyl Parathion	38.4	33.3	33.5	37.2	52	60	66	52
Chlorine	38.2	33.1	36.5	35	53	61	58	61
Ethylene oxide	38.2	41.4	37.4	46.7	54	39	56	33
Cumene	37.8	32.8	41.6	31.4	55	62	43	68
1,2-Dichloroethane	37.7	40.9	38.4	43.7	56	43	53	38
Cyclohexane	37.4	32.4	37.1	31.1	57	63	57	70
Bis(2-ethylhexyl) adipate	36.7	31.8	41.4	26.7	58	64	44	91
Phenol	35.9	31.1	31.5	37.9	59	65	71	50
Di-n-octyl phthalate	35.8	31	40.4	26	60	66	45	92
Phosphoric acid	35.4	30.7	29.4	36.1	61	67	82	57
Malathion	35.4	30.6	32.7	32.1	62	68	68	67
Cresol (mixed isomers)	35.3	30.5	31.3	35.2	63	70	73	58
Phosphorus (yellow or white)	35.2	30.5	35.2	30.9	64	71	63	73

TOTAL HAZARD VALUES AND CHEMICAL RANKS, NOT WEIGHTED BY RELEASES

Chemical	Hazard value				Chemical rank			
	Even weight	Double carcin. weight	Half human acute	Half environ. weight	Even weight	Double carcin. weight	Half human acute	Half environ. weight
Acrylonitrile	35.2	36.1	34.7	37.1	65	54	64	53
p-Cresol	35.1	30.4	29.8	35	66	73	80	60
Carbon tetrachloride	34.8	39.1	38.6	36.8	67	44	52	54
4,4'-Isopropylidenediphenol	34.7	30.1	33	30.5	68	74	67	74
Chlorophenols [o]	34.6	30	30.3	33.5	69	75	78	64
Chloroform	34.5	38.2	36.4	38	70	47	60	49
Benzene	34.4	41	38.8	36.8	71	42	51	55
1,4-Dichlorobenzene	33.2	37.3	34.2	34.6	72	51	65	62
p-Xylene	33.1	28.6	36.3	27.1	73	77	61	89
Hydrochloric acid	32.7	28.4	30.7	30.9	74	79	75	72
Chlorine dioxide	32.5	28.2	31.4	30.2	75	80	72	77
Barium compounds	32.3	28	31.7	31.4	76	81	69	69
Atrazine	31.7	27.5	29.7	28.4	77	83	81	84
Toluene-2,4-diisocyanate	31.4	34.5	28.7	36.1	78	57	84	56
Chlorobenzene	30.8	26.7	30.6	29.1	79	85	76	80
Cyanazine	30.5	26.4	27.1	29	80	86	92	81
Cumene hydroperoxide	30.4	28.6	26.6	31.1	81	78	98	71
N,N-Dimethylaniline	30.2	26.1	29	30.5	82	87	83	76
Picric acid	30	26	27.2	27.9	83	88	91	86
Molybdenum trioxide	29.7	25.7	30.8	29.4	84	90	74	79
Manganese compounds	29.7	25.7	28.7	29.7	85	89	85	78
Bromomethane	29.3	25.4	28	28.2	86	91	89	85
Ethylbenzene	28.8	25	31.6	26	87	93	70	93
Metam Sodium (MeNHCS2Na)	28.5	24.6	28	23.8	88	94	88	101
1,2,4-Trimethylbenzene	28.4	24.6	30.4	21	89	95	77	107
Methylenebis(phenylisocyanate)	28	24.3	23	28.9	90	96	107	83
Aniline	27.7	24	23.8	28.9	91	97	105	82
Xylene (mixed isomers)	27.4	23.7	30.2	24.8	92	98	79	96
Acetaldehyde	26.7	30.6	26.9	27.4	93	69	95	87
Alachlor	26.4	22.9	28.2	19.6	94	99	87	112
Catechol	26.3	22.8	26.7	21.2	95	100	97	106
Propionaldehyde	26.3	29.2	27.3	27	96	76	90	90

TOTAL HAZARD VALUES AND CHEMICAL RANKS, NOT WEIGHTED BY RELEASES

Chemical	Hazard value				Chemical rank			
	Even weight	Double carcin. weight	Half human acute	Half environ. weight	Even weight	Double carcin. weight	Half human acute	Half environ. weight
o-Xylene	26	22.5	28.3	24	97	101	86	99
Carbaryl	25.4	22	27	23.7	98	103	93	102
Propylene oxide	25	27.7	25.4	30.5	99	82	99	75
m-Xylene	24.7	21.4	26.8	21.6	100	104	96	104
1,1,1-Trichloroethane	24.3	21.1	25.2	24.6	101	106	100	97
EPTC (ethyl dipropylthiocarbamate	24.1	20.8	24	19.8	102	107	104	111
Zinc compounds	23.8	20.7	27	15.9	103	108	94	128
Acrylic acid	23.3	20.2	20.4	24.2	104	109	115	98
Butyl acrylate	23.1	20	24.4	17.4	105	110	102	121
Butyl benzyl phthalate	22.3	19.3	24.2	18.1	106	111	103	120
Allyl chloride	22.1	21.3	21.4	24	107	105	109	100
Maneb	22	19.1	24.8	19	108	112	101	114
Carbon disulfide	21.4	18.6	20.6	27.1	109	113	114	88
Butylate	21	18.2	23.7	14.1	110	115	106	132
Chloroethane	20.6	17.8	17.6	20.4	111	116	123	109
Benzoyl chloride	19.7	17.1	18.1	20.4	112	117	120	108
Metolachlor	19.4	16.8	21.3	13.7	113	118	110	134
Dichloromethane	19.4	25.1	20.6	22.6	114	92	113	103
Asbestos (friable)	19.2	30.5	21.7	25.6	115	72	108	94
Toluene	19.2	16.6	21.1	17	116	119	111	125
Isopropyl alcohol	18.9	27.4	21.1	24.8	117	84	112	95
Diethyl phthalate	18.9	16.4	17.6	17	118	120	122	124
Nitrobenzene	18.7	16.2	19	18.3	119	121	118	117
Pyridine	18.5	16	16.9	18.8	120	122	124	115
Hydroquinone	18.1	15.7	17.6	17.1	121	123	121	123
Propylene	17.8	15.4	20.1	11.9	122	125	116	139
Terephthalic acid	17.4	15.1	19.7	13.7	123	126	117	133
Ethylene	16.7	14.5	18.9	12.8	124	127	119	137
2-methoxyethanol	16.7	14.4	15.4	20.2	125	128	126	110
Maleic anhydride	16.1	18.4	14.6	19.5	126	114	130	113
Zinc (fume or dust)	16	13.9	14.5	21.3	127	129	132	105
Vinyl acetate	15.7	13.6	15.3	15	128	130	127	130

TOTAL HAZARD VALUES AND CHEMICAL RANKS, NOT WEIGHTED BY RELEASES

Chemical	Hazard value				Chemical rank			
	Even weight	Double carcin. weight	Half human acute	Half environ. weight	Even weight	Double carcin. weight	Half human acute	Half environ. weight
Isobutyraldehyde	15.2	13.2	16.1	13.1	129	131	125	136
Dimethyl phthalate	15.1	13.1	12.7	15.3	130	132	136	129
Chloromethane	14.9	15.5	14.8	18.3	131	124	129	118
2-ethoxyethanol	14.8	12.8	14	18.2	132	133	133	119
Phthalic anhydride	14.7	12.7	13	17.3	133	134	135	122
1,4-Dioxane	14.6	22.3	15.2	18.7	134	102	128	116
Diethanolamine	13.8	12	9.8	16	135	135	142	127
Butyraldehyde	13.8	12	14.6	10.4	136	136	131	143
Methyl ethyl ketone	12.9	11.2	13.5	16.5	137	137	134	126
Glycol ethers	12.1	10.4	8.3	14.3	138	138	144	131
Methyl methacrylate	11.5	10	12.6	13.2	139	139	137	135
1,2-Dichloropropane	10.7	9.3	10.7	8.8	140	140	139	145
Methyl isobutyl ketone	10.6	9.1	10.4	12.2	141	141	141	138
n-butyl alcohol	9.8	8.5	8.9	10.8	142	142	143	141
Metribuzin	9.6	8.3	10.8	6.4	143	143	138	149
Antimony compounds	9.3	8.1	10.5	10.7	144	144	140	142
Aluminum (fume or dust)	8.3	7.2	4.7	11.1	145	145	150	140
Ethylene glycol	7.6	6.6	5.7	10.1	146	146	149	144
Thorium dioxide	6.8	5.9	5.8	6.8	147	147	148	147
Ammonium nitrate (solution)	6.3	5.5	7	6.5	148	148	145	148
Freon 113	5.8	5	6.6	5.7	149	149	146	150
Acetonitrile	5.6	4.8	6.1	7.2	150	150	147	146
Acetone	4.3	3.7	4.4	5.1	151	151	151	151
Carbonyl sulfide	3.2	2.8	3.6	4.3	152	152	152	152
Methanol	2.5	2.2	2.9	3.4	153	153	153	153
Ammonium sulfate (solution)	2.4	2.1	2	2.4	154	154	154	155
tert-butyl alcohol	2.3	2	1.8	2.5	155	155	155	154
Methyl tert-butyl ether	1.6	1.4	1.5	1.4	156	156	156	156
Glyphosate	1	0.9	1.1	0.7	157	157	157	157
sec-butyl alcohol	0.5	0.4	0.3	0.7	158	158	158	158

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