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Office of Pesticides
and Toxic Substances
Washington, DC 20460

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Toxic Substances

# Chemical Selection Methods: An Annotated Bibliography

## *Second Edition*

## Toxics Integration Information Series

Toxics Integration Information Series

EPA 560/TIIS-83-003
March, 1983

# Chemical Selection Methods: An Annotated Bibliography

Second Edition

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## FOREWORD

The selection, ordering, and ranking of chemical substances stands as one of the most critical, yet difficult, tasks facing those who are engaged in the testing, assessment, and regulation of substances as well as enforcement of those regulations. The Office of Toxics Integration has discovered a number of resource materials that might serve the needs of those in other federal agencies as well as those in states, industry, and academia. This annotated bibliography is intended to assist those faced with decisions related to the selection of chemicals to become aware of the state-of-the-art for those decision-making processes. Hopefully, duplicative and overlapping efforts can be avoided through such awareness.

We anticipate further updating of this bibliography. Your comments, suggested revisions, and additions should be addressed to: Office of Toxics Integration, TS-777, U.S. Environmental Protection Agency, 401 M Street, SW, Washington, DC 20460, telephone (202) 382-3393. Copies of all materials referenced in this bibliography are available for examination.

Walter W. Kovalick Jr.

Walter W. Kovalick, Jr.
Acting Director
Office of Toxics Integration

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## OTHER PUBLICATIONS IN THE TOXICS INTEGRATION POLICY SERIES:

State Administrative Models for Toxic Substances Management (July 1980)
EPA-560/13-80-018: PB81-147373

State Integrated Toxics Management: Fact and Challenge (July 1981)
EPA-560/TIPS-81-001; PB81-242406

Chemical Substances Designation (December 1981)
EPA-560/TIIS-82; PB83-130294

## OTHER PUBLICATIONS IN THE TOXICS INTEGRATION INFORMATION SERIES:

EPA Chemical Activities Status Report - 1st Edition (June 1979)
EPA-560/13-79-003

EPA Chemical Activities Status Report - 2nd Edition (December 1980)
EPA-560/13-80-040(a), PB81-176414; EPA-13-80-040(b), PB81-176422

EPA Chemical Activities Status Report - 3rd Edition (June 1982)
EPA-560/TIIS-82-002a, -002b

Chemical Substances Designation (December 1981)
EPA-560/TIIS-82-003, PB83-130294; -004, PB83-130302; -005, PB83-130310; -006; PB83-130328

Directory of Federal Coordinating Groups for Toxic Substances - 1st Edition (June 1979) EPA-560/13-80-008; PB80-137870

Directory of Federal Coordinating Groups for Toxic Substances - 2nd Edition (March 1980) PB80-177314

Perspectives on the Top 50 Production Volume Chemicals (July 1980)
EPA-560/13-80-27; PB80-221682

Federal Activites in Toxic Substances (May 1980)
EPA-560/13-80-015 Revised May 1983; PB-157638

TSCA Status Report for Existing Chemicals Volume 1, Issue 2 (July 1980)
EPA-560/13-80-033

TSCA Status Report for Existing Chemicals Volume 2, Issue 2 (July 1981)
EPA-560/TIIS-81-004

Perspectives on State-EPA Grant Activities (September 1980)
EPA-560/13-80-037; PB82-229105,

Chemical Selection Methods: An Annotated Bibliography (November 1980)
EPA-560/TIIS-80-001; PB81-241481

Chemical Information Resources Handbook (January 1981)
EPA-560/TIIS-81-002; PB82-225657

Toxic Substances Control Act Grants to States (July 1981)
EPA-560/TIIS-81-003; PB81-232969

TSCA Chemicals in Commerce Inventory: Regional and State Perspectives
(August 1981) EPA-560/TIIS-81-005

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National Technical Information Service
4285 Port Royal Road
Springfield, VA 22161

# INTRODUCTION

This bibliography is intended to provide individuals interested in chemical selection (priority setting, ranking, indexing, sorting) with a collection of relevant materials. Examining such materials may prevent unnecessary duplication of effort and aid in developing new methods to help select chemicals of concern. The selection methods listed here were developed by the EPA, other federal agencies, state agencies, and contractors for these agencies, as well as industrial, academic, and public interest organizations.

Included with each entry is a brief abstract. Some of the abstracts were prepared specifically for this effort; others accompanied the original documents. This second edition adds 15 new citations to the original report; these new citations are asterisked in the Author Index.

Chemical selection has been and continues to be of interest to many groups concerned with the assessment and regulation of toxic substances. For example, the Toxic Substances Control Act (Public Law 94469) requires the EPA to compile an inventory of chemical substances manufactured, imported, or processed in the United States for commercial purposes.[1] By June 1982, over 70,000 chemicals were included in this Inventory. The EPA is also responsible for determining which of these chemicals may require testing, which should be subject to information-gathering rules and which might require regulatory controls. Making these types of determinations requires "selecting" small groups of substances from larger groups.

Because of the large number of potentially toxic substances and the variety of actions possible under numerous federal and state authorities, the development and use of systematic selection methods has become necessary. Of course, use of systematic selection methods is appropriate only at certain stages in decision processes affecting chemicals. For example, early in any process, candidates must be screened to identify substances clearly requiring some assessment; later, candidates from the first group must be chosen for more in-depth consideration; and, finally, a few candidates are selected for intensive analysis. Thus, selection methods can be applied to candidate pools that are large or small and to information ranging from limited to extensive. However, selection schemes must be developed and employed "operationally," that is, with regard to the requirements of the particular stage in the decision-making process that is being considered.

## Limitations

There are also some inherent limitations in the use of any chemical selection method. Most selection methods involve consideration of some or all of the following factors: carcinogenicity, mutagenicity, teratogenicity, neurotoxicity, and other chronic human health effects; acute human health

[1] Excluded from this inventory are mixtures, pesticides, tobacco, food, food additives, drugs, cosmetics, firearms, and nuclear materials.

effects; environmental toxicity; types and quantities of emissions and environmental exposure; bioaccumulation; costs of regulation; and regulatory authority. Any method that involves combining various categories of information to arrive at some single index of concern risks obscuring the problems created by the original data.

Existing systematic selection methods generally use some form of scoring or ranking which involves assigning a dimensionless or arbitrary number to each of the factors being considered. Conversions of this type, while summarizing large amounts of information, also tend to obscure the original information, and fail to incorporate a measure of uncertainty. Suppose, for example, that the number "3" is assigned to any substance to which between 10,000 and 100,000 persons are exposed. Not only will this number fail to convey accurately the number exposed, it will also fail to provide an indication of the level of uncertainty in the estimate or an indication of the basis for the estimate (e.g., monitoring, modeling).

Another limitation to the use of many scoring methods is that they employ simple additive or multiplicative algorithms to combine factors. Such algorithms often ignore or distort the true relationship between factors. In the case of an additive system, suppose that for Chemical X, carcinogenicity is assigned a "5", no information is available for six other factors so each is assigned a "0", and persistence is assigned a "3". The total score for Chemical X is "8". For Chemical Y, carcinogenicity is assigned a "1", each of six other factors is also assigned a "1", and persistence is assigned a "3". Thus, the total score for Chemical Y is "10". It is unclear, however, whether Chemical Y is really deserving of more intensive review than Chemical X, regardless of the policy framework governing the evaluator.

Some methods utilize "flagging" or "triggering," as a means of selection. "Flagging" refers to setting threshold levels or employing "discriminators" for various factors in order to select candidates. Any chemical may be "flagged" if it exceeds the discriminators for certain combinations of factors. The use of "flags" or "triggers" in a selection scheme avoids the complex data manipulations required for the systems discussed above. However, selection methods using "flagging" are only effective if the factors are chosen carefully.

System Comparisons

It is beyond the scope of this work to perform a comprehensive review and critique of past priority scoring systems developed for use in selecting chemicals for study and/or possible regulatory action in other contexts. However, Table 1 summarizes the number and types of variables used in several different systems. In general, these few selected systems were designed to accommodate a wide variety of information. Three of the systems call for scoring more than two dozen different variables.

Table 1

NUMBER AND TYPES OF FACTORS CONSIDERED
(Numbers represent the number of variables within each category.)

| System | Production or release | Exposure | Biological Responses | | | Multi-media character | Total factors scored |
|---|---|---|---|---|---|---|---|
| | | | for humans* | Other | Total | | |
| A | 1 | 2** | 5 | 0** | 5** | 1****** | 9 |
| B | 7***** | 9*** | 5 | 5 | 10 | 0 | 26 |
| C | 0 | 2*** | 6 | 1 | 7 | 0 | 9 |
| D | 2 | 0 | 3 | 1 | 4 | 0 | 9**** |
| E | 4 | 12 | 6 | 3 | 9 | 0 | 25 |
| F | 1 | 14 | 6 | 4 | 10 | 0 | 25 |

*In cases where the scoring factor could apply either to humans or to a larger group of animals (e.g., "terrestrial animals"), it was counted as applying to humans. The only factors considered under "other" were those that could not include human data, such as plants and aquatic animals.
**Bioaccumulation, 1 of the 2, was treated by the system as an exposure variable.
***Persistence and bioaccumulation were counted here as exposure variables, although they were treated on par with response variables in the system.
****Included three miscellaneous variables (ignitability, reactivity, corrosivity) that relate to neither production, exposure, nor biological effects.
*****Included production, consumption, imports, exports, and release to various specific environmental media.
******A factor was included that gave extra points if other agencies had standards for the chemical being scored.

Table 2 compares some general properties of the systems surveyed. The first column (ranking vs. screening as the overall approach) distinguishes systems that are intended to rank a number of candidates for action from systems that use a series of screens (pass/fail tests) arranged in a decision tree to select a group of candidate chemicals that meet a specified set of criteria. The second column discusses the method for computation of final scores. All but one system had some provision for doing this, usually based on derived scores rather than raw data.

The final column of Table 2 represents an independent assessment of the need for research-level expertise. Generally, the criterion for this judgment was that if the system required extensive evaluation of raw research results in a particular field, it would usually be necessary to have a Ph.D. or equivalent in that field involved in some way in at least checking the analysis.

## Summary

Systematic selection methods will certainly continue to be significant in the selection of chemicals for assessment and regulation. Such methods can provide consistency in decision-making. They also can promote efficient resource allocation. Finally, use of these methods can aid in the defensibility and effectiveness of regulatory actions.

The selection schemes presented in this publication range from quite simple to very sophisticated and, with minor tailoring, can be adapted to virtually any chemical selection need. This publication is intended to provide quick reviews of many approaches to chemical selection, with the hope that an early overview will save time and money for those wishing to select or create a system of their own.

Table 2

GENERAL PROPERTIES OF THE PROCEDURE FOR ARRIVING AT FINAL SCORES

| System | Ranking or screening as overall approach | Selected properties | Overall expertise required |
|---|---|---|---|
| A | Ranking | Uses only derived scores. Related factors grouped into "components"; components combined in various ways (e.g., addition, multiplication). Component scores normalized, weighted, and aggregated to form final score. | Ph.D. or equivalent in one specialty (biology) |
| B | Ranking (within components) | Uses raw data for production/release, but derived scores for all other factors. Authors opposed combining scores because of different scales used. | Ph.D. or equivalent in many specialties |
| C | Ranking, but screening at end | Uses only derived scores. Scores combined by addition. | Ph.D. or equivalent in many specialties (aquatic biology, environmental transport, toxicology, carcinogenesis, genetics) |
| D | Screening/ Selection | Uses quantitative data cut-off for production/release, but derived scores for biological response. Yes/no decision tree used to select substances; no scores combined. | Ph.D. or equivalent in one specialty (biology) |
| E | Ranking followed by a sort into three "zones" of overall hazard | Uses quantitative data exclusively. Each factor's data added or multiplied; some factors weighted. | Ph.D. or equivalent in many specialties |
| F | Ranking (within components) | Uses only derived scores. Addition of factor scores into four "component" scores; these scores normalized. No further aggregation of component scores, so no final score for each substance. | Ph.D. or equivalent in many specialties |

# Chemical Selection Methods

Allport, J.; Casey, S.; Cook, J.; et al.
Stanford Research Institute, Menlo Park, California
A Study of Industrial Data on Candidate Chemicals for Testing--Final Report
Prepared for U.S. Environmental Protection Agency
Office of Toxic Substances
EPA-560/5-77/006, Research Request No. 1
NTIS #PB-274 264/1GA, 1977

This report summarizes the work done by Stanford Research Institute for EPA's Office of Toxic Substances and includes three major parts. (1) Data previously collected on a NSF study were supplemented to provide the following information, where available, on 667 industrial chemicals: (a) United States production; (b) estimates of quantities released annually to the environment; (c) major uses; and (d) references on mutagenicity tests. Mutagenicity data on 25 chemicals were evaluated after developing a list of assays and criteria for classifying the results as either positive or negative/inadequate. (2) Tables which contain economic information on 1,791 chemicals belonging to 26 structural classes considered to represent potential industrial carcinogens and mutagens were prepared. For those chemicals with annual production greater than one million pounds, market forecasts which present a brief summary of production, consumption patterns, major uses, possible substitutes, and growth trends were prepared. (3) Carcinogenicity data for all chemicals belonging to three classes (epoxides, alkyl halides, and vinyl halides) were used to correlate structural features with carcinogenic activity. Criteria were developed for estimating the potential carcinogenicity of chemicals in each class. These criteria were applied to those chemicals in each class known to be produced commercially or for which there was evidence of significant human exposure. The results of the study were summarized in three separate reports.

Ross, R.H.
Oak Ridge National Laboratory
Welch, J.
U.S. Environmental Protection Agency, Office of Toxic Substances
Proceedings of the EPA Workshop on the Environmental Scoring of Chemicals
Washington, D.C., August 13-15, 1979
EPA-560/11-80-010, May 1980

The environmental scoring of chemicals is viewed by the EPA as a tool to assist in the ranking or ordering of the universe of chemicals that are under the jurisdiction of the Toxic Substances Control Act. The purpose of scoring is to identify most of the chemicals that have a high probability for requiring review for regulation or testing. This report describes a 3-day workshop held in Washington, D.C., August 13-15, 1979, to develop an environmental scoring system. Initial discussions centered on the determination of a safety factor (calculated as the concentration at which an effect is observed divided by environmental concentration) that would allow a numerical score to be assigned to a chemical to reflect its potential hazard. Further discussion, however, indicated that the environmental concentration of a chemical is usually not available and that the estimation of an environmental concentration is not readily accomplished; therefore, a scoring system was developed that does not require environmental concentrations. This system relates environmental exposure to toxicity by using a multiplier (3x, 2x, or 1x) which is assigned on the basis of the concentration at which an effect is observed. The applicability of the scoring system is demonstrated by scoring selected chemicals.

Flinn, J.E.; Thomas, T.J.; Bishop, M.D.
Battelle Columbus Laboratories
Columbus, Ohio
Identification Systems for Selecting Chemicals or Chemical Classes as Candidates for Evaluation
Prepared for U.S. Environmental Protection Agency
Office of Toxic Substances
EPA-560/1-74/001
NTIS #PB-238 196/OGA, November 1974

This report is a review of various systems for selecting, assessing, and ranking chemicals for their health and environmental effects. Systems for two general areas are considered: health planning, including environmental, occupational, and general health; and environmental management. It is noted that the term "system" is broadly defined to include not only formalized organizational structures, models, and methodologies, but also less formal tools, methods, and working groups which have been created to rank chemical substances or effects. Existing systems are classified in several ways. Some are considered information repositories for chemical data, particularly toxicity data. Other systems are classified with respect to whether their function is to identify chemical substances before or after general exposure of the public and the environment occurs. Each of these types is further categorized into those which identify new or unrecognized chemical "stressors" and those which evaluate recognized "stressors." Particular attention is given to methods used by various federal agencies. It is concluded that most existing systems are deficient in that they focus on acute rather than long-term effects; have a limited domain of concern; and are not designed to identify hazards from degradation products, synergistic effects, or effects on the nonliving environment. An appendix summarizes results of a seminar on "Early Warning Systems for Toxic Substances" held January 30 - February 1, 1974.

Venezian, E.C.
Arthur D. Little, Inc.
Cambridge, Massachusetts
Pre-screening for Environmental Hazards - A System for Selecting and Prioritizing Chemicals
Prepared for U.S. Environmental Protection Agency
Office of Toxic Substances
Washington, D.C.
EPA/560/1-77/002, April 1977

Alternatives were considered for prescreening chemicals to assess their potential environmental hazard. A system design concept which takes into account both the toxicity of the chemical and the eventual levels which it can be expected to reach in the environment was selected for further analysis. It is noted that, although neither toxicity nor eventual levels can be predicted with great accuracy, the accuracy attainable by simple methods appears adequate for selecting and ranking chemicals for additional investigation. A specific design which relies on data which are usually available was developed to the point of testing the feasibility of collecting the necessary data and performing the required computations on five chemicals.

TSCA Interagency Testing Committee: Initial Report to the Administrator, Environmental Protection Agency
42 FR 197:55026-80, October 1977

Section 4(e) of the Toxic Substances Control Act (TSCA) requires the establishment of a committee to identify and recommend to the EPA Administrator chemical substances which should be tested to determine their hazard to human health or the environment. This report documents procedures used by the TSCA Interagency Testing Committee for selecting those chemical substances recommended for testing. Reasons for each recommendation are outlined. Available data and potential data for carcinogenic, mutagenic, teratogenic, and chronic toxic effects were all considered, as was the ability of the substances to bioaccumulate or cause deleterious environmental effects. A scoring system which took into account both available information and the lack of it for these factors was used in the screening process. Categories or substances recommended for further testing include alkyl paraffins, chloromethane, cresols, hexachloro-1,3-butadiene, nitrobenzene, toluene, and xylenes. The formation of the Interagency Testing Committee, its responsibilities, and the approach used in forming the recommendations are discussed. Sources of data used in the preparation of the initial substances list are given. A linear weighting scheme used to rank the substances is discussed.

Enviro Control Inc.
Rockville, Maryland
Scoring Chemicals for Health and Ecological Effects Testing
Proceedings of TSCA-ITC Chemical Scoring System Workshop
February 25-28, 1979

Since its inception in early 1977, the Toxic Substances Control Act Interagency Testing Committee has submitted to the EPA Administrator four reports recommending a total of 33 chemicals and chemical categories to be tested for their potential to cause unreasonable risk to human health or the environment. In order to identify these chemicals from among the approximately 44,000 chemicals in commercial production in the United States today, it was essential for the Committee to have procedures for ranking chemicals as to the need for testing to determine their hazard to human health and the environment.

The Committee used existing source lists of hazardous chemicals to form a Master File, as described in the Committee's Initial Report to the Administrator. This list of 1,700 chemicals was subjected to scoring, first on the basis of production, release, operation, and exposure, and subsequently on the basis of biological activity. The scoring procedure was developed in conjunction with Clement Associates, Inc., the Committee's support contractor during its first 2 years of operation, and is described in this report.

In an effort to make any possible improvement in this numerical scoring system, the Committee decided to subject the scoring system to the scrutiny and criticism of individuals from academia, industry, and government who were expert in the various aspects of release, exposure, and effects that comprise the system. Enviro Control, Inc. was awarded a contract to organize a scoring workshop and to prepare a report on the proceedings. The workshop was held in San Antonio, Texas, February 25-28, 1979, with approximately 80 technical experts participating.

Fuller, B.; Hushon, J.; Kornreich, M.; et al.
Mitre Corporation, McLean, Virginia
Preliminary Scoring of Selected Organic Air Pollutants, 5 Volumes
Prepared for U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina
EPA-450/3-77/008a,b,c,d,e
NTIS #PB-264 442/5ST, October 1976

This report presents a scheme for evaluating the relative hazard to humans resulting from air emissions during production of synthetic organic chemicals. Data on production, fraction lost during production, volatility, and toxicity have been compiled for 637 organic chemicals. A scoring system using these data elements was developed and is described in this report. Scores assigned to the 637 chemicals are presented. Four appendices were published with this report. The appendices are dossiers containing chemistry, production, and toxicity data for the 637 synthetic organic chemicals.

Fiksel, J.; Segal, M.
Arthur D. Little, Inc.
An Approach to Prioritization of Environmental Pollutants: The Action Alert System -- Final Draft
Prepared for U.S. Environmental Protection Agency
Office of Water Regulations and Standards
Monitoring and Data Support Division
Washington, D.C.
Contract No. 68-01-3857, June 1980

The Action Alert System was developed to assist the Office of Water Regulations and Standards in evaluating available data, setting priorities, and determining appropriate actions. The system can aid in sorting large groups of chemicals into "manageable clusters" for further examination.

The two required data elements are (1) concentrations, including drinking water, human diet, and ambient water; and (2) effects data, including chronic mammalian, acute human or mammalian, and aquatic toxicity. Six auxiliary modules have been developed to serve as surrogates in cases where data are lacking or to enable use of more extensive data where they exist. This report includes a detailed description of the conceptual development of the system, a presentation of the six auxiliary modules, and a user's guide. The user's guide provides detailed instructions for the application of the Action Alert System to the ranking of specific chemicals.

Dorsey, J.A.; Johnson, L.D.; Statnick, R.M.; et al.
Environmental Assessment Sampling and Analysis: Phased Approach and Techniques for Level 1
Prepared for U.S Environmental Protection Agency
Industrial Environmental Research Laboratory
Research Triangle Park, North Carolina
EPA-600/2-77/115
NTIS #PB-268 563/4ST, June 1977

The report discusses a three-level approach to sampling and analysis for environmental source assessment. A research program was initiated to develop a sampling and analytical approach for conducting environmental source assessments of the feed, product, and waste streams associated with industrial and energy processes. An environmental source assessment identifies potential air, water, and terrestrial problems for both regulated and unregulated pollutants. The three-level sampling and analysis approach resulted from this program. Level 1 is a complete survey of all streams, using simplified, generalized sampling and analytical methods which permit priority ranking; i.e., hazardous streams are distinguished from those less hazardous or relatively innocuous in nature. Level 2 is detailed sampling and analysis of the streams ranked in the highest priority by the Level 1 survey. Other streams may then be addressed according to potential hazard. Level 3 involves continuous monitoring of "key" indicator materials to evaluate the effect on emissions of process variability.

Archer, S.R.; McCurley, W.R.; Rawlings, G.D.
Monsanto Research Corporation, Dayton, Ohio
Source Assessment: Pesticide Manufacturing Air Emissions--Overview and Prioritization
Prepared for U.S. Environmental Protection Agency
Industrial Environmental Research Lab
Research Triangle Park, North Carolina
EPA-600/2-78/004d
NTIS #PB-279 171/3ST, March 1978

This report is an overview of the pesticide manufacturing industry and ranks 80 major pesticides based on their potential environmental burden from an air pollution standpoint. Production of synthetic organic pesticides was about 640,000 metric tons in 1974. Thirty-seven major synthetic organic pesticides, those with annual production of 4,540 or more tons, accounted for 74% of the market. Elemental chlorine is common to most pesticides, but other raw materials include hydrogen cyanide, carbon disulfide, phosgene, phosphorus pentasulfide, hexachlorocyclopentadiene, various amines, and concentrated acids and caustics. Air pollution aspects of the pesticide manufacturing industry are essentially without quantitative data. For some plants, the pollution caused by loss of active ingredients is less significant than that caused by unreacted by-products. Evaporation from holding ponds and evaporation lagoons may also be an emission source, although few quantitative data are available. Emissions emanate from various pieces of equipment and enter the atmosphere as both active ingredients and as raw materials, intermediates, and by-products. Air emission control devices include baghouses, cyclone separators, electrostatic precipitators, incinerators, and gas scrubbers. Synthetic organic pesticide production in 1985 will be about 806,000 metric tons.

Brown, S.L.; Holt, B.R.; McCaleb, K.E.
Stanford Research Institute, Menlo Park, California
Systems for Rapid Ranking of Environmental Pollutants: Selection of Subjects for Scientific and Technical Assessment Reports
Prepared for U.S. Environmental Protection Agency
Office of Research and Development
Office of Health and Ecological Effects
Washington, D.C.
EPA-600/5-78/012
NTIS #PB-284 338/1ST, June 1978

This document reports the results of the development and testing of a system for rapidly ranking environmental pollutants. One potential use for the system is in choosing the most important candidates for Scientific and Technical Assessment Reports (STAR). Of several possible approaches to ranking environmental agents, a system depending on expert opinion but assisted by an objective subsystem was selected for development. The system defines procedures for collecting, processing, and evaluating data on production and use; environmental transport, transformation, and rate; and human health welfare and ecological effects. A test of the objective subsystem confirmed the utility of the system. Of ten candidate agents, the three highest ranked were cyanides, carbon disulfide, and beryllium.

Stacey, G.S.; Flinn, J.E.
Battelle Columbus Labs, Ohio
Development of an Economics-Based Methodology for Projecting Future Pollution Problems
Prepared for U.S. Environmental Protection Agency
Office of Research and Development
Office of Health and Ecological Effects
Washington, D.C.
EPA-600/5-78/011
NTIS #PB-284 337/3ST, June 1978

The report describes a project designed to develop a methodology for identifying potential future toxic substance pollution problems. An approach was desired that would be systematic, comprehensive, and futuristic. The methodology developed is based on exposure and initiates the identification of problems by focusing on the potential for their occurrence in the production, exchange, and consumption of goods and services. Products are ranked according to the potential they have for being associated with future pollution problems. For the high-ranked products, additional information on the chemical constituents of the product are identified. The final step is to analyze the chemical constituents to determine which chemicals occur frequently and in large quantities. At the same time the potential that each of the chemicals has for resulting in toxic substance problems would be assessed. In ranking the products, parameters concerning historical growth, future growth, dispersion, technical change, and value of shipments were developed and applied. A specific group of products was examined to determine their chemical content. The results of this effort showed that identifying chemical constituents of products required considerable resources. The final step of analyzing chemicals to determine frequency and quantity was developed conceptually, but, due to resource limitations, could not be applied.

Cleland, J.G.; Kingsbury, G.L.; Sims, R.C.; White, J.B.
Research Triangle Institute
Research Triangle Park, North Carolina
Multimedia Environmental Goals for Environmental Assessment. 4 Volumes
Prepared for U.S. Environmental Protection Agency
Industrial Environmental Research Laboratory
Research Triangle Park, North Carolina
EPA-600/7-77/136a, EPA600/7-77/136b, EPA600/7-79/176A, EPA600/7-79/176B
NTIS #PB-276 919/8ST, #PB-276 920/6ST, #PB80-115108, #PB80-115116, August 1979

The report gives results of a study of the derivation of Multimedia Environmental Goals (MEG's). MEG's are levels of significant contaminants or degradents (in ambient air, water, or land, or in emissions or effluents conveyed to the ambient media) that are judged to be either appropriate for preventing certain negative effects in the surrounding populations or ecosystems or representative of the control limits achievable through technology. In the context of deriving MEG's, Volume I: offers perspective on the broad range of contaminants whose control is vital to both industry and the public; further develops and defines indicators designating contaminants which must be given priority consideration for immediate control and for subsequent research; brings existing and emerging data together for use in environmental assessment; and explores some basic methodologies which provide the present MEG's, and which also suggest directions for refined methodologies. MEG's are projected for more than 650 pollutants. Of these, 216 substances receive full attention in Volume II. MEG charts along with the Background Information Summaries for these substances are presented in this volume which includes 162 organic and 54 inorganic substances. Volumes III and IV address 586 organic compounds. Volume III includes the following categories: Aliphatic Hydrocarbons; Alkyl Halides; Ethers, Halogenated Ethers, and Epoxides; Alcohols; Glycols and Epoxides; Aldehydes and Ketones; Carboxylic Acids and Derivatives; Nitriles; Amines; Azo Compounds, and Hydrazine Derivatives; and Nitrosamines. Volume IV includes the following categories: Thiols, Sulfides and Disulfides; Sulfonic Acids and Sulfoxides; Benzene and Substituted Benzene Hydrocarbons; Halogenated Aromatic Compounds; Aromatic Nitro Compounds; Phenols; Halogenated Phenolic Compounds; Nitrophenols; Fused Polycyclic Hydrocarbons; Fused Non-alternant Polycyclic Hydrocarbons; Heterocyclic Nitrogen Compounds; Heterocyclic Oxygen Compounds; Heterocyclic Sulfur Compounds; and Organophosphorus Compounds.

Pielmeier, G.R.
Tracor Jitco, Inc.
Rockville, Maryland
Identification of High Risk Occupational Groups and Industrial Processes Using RTECS/NOHS Data--Final Report
Prepared for U.S. Department of Health, Education and Welfare
Public Health Service
Center for Disease Control
National Institute for Occupational Safety and Health
Division of Surveillance, Hazard Evaluations and Field Studies
Cincinnati, Ohio
Contract No. 210-78-0076, November 1979

Two NIOSH data files, the Registry of Toxic Effects of Chemical Substances and the National Occupational Hazard Survey, contain data that pertain to the risk posed to workers by toxic chemicals in the workplace. In order that occupationally and industrially defined groups of workers at high risk might be identified and given their proper priorities in NIOSH activities, algorithms were developed which combine data from the two data files identified above, produce indexes of the potential risk to workers in specific occupations and industries, and rank the chemicals to which workers are exposed in terms of their toxicological hazard and their potential risk to all workers. The steps involved in development of these algorithms are described in this report. Five indexes are developed: (1) Hazard Risk Index, (2) Adjusted Hazard Risk Index, (3) Occupational Risk Index, (4) Industry Risk Index, and (5) Occupation within Industry Risk Index. Representative pages from the indexes are presented.

Stanford Research Institute
Menlo Park, California
Criteria and Procedures for Chemical Selection
Prepared for Chemical Selection Working Group, National Cancer Institute, Bethesda, Maryland
Contract: NO1-CP-95607, October 1977

This report describes the criteria and procedures used by the Chemical Selection Working Group to select chemicals for NCI's carcinogenesis bioassay program. Chemicals are nominated for consideration by a variety of government agencies and others. A two-step process is then used for selection. The first step involves gathering limited data to determine if the chemical meets qualifying criteria. In order to qualify, a chemical must: not currently be undergoing testing by the NCI bioassay program or other programs; not have been adequately tested previously; and have high annual consumption or evidence of exposure from environmental occurrence. If the chemical meets these criteria, more extensive selection criteria are then applied. This step involves analyses of: exposure information, including consumption, use patterns, human exposure, and environmental occurrence; and evidence for possible carcinogenic activity, including human data, animal data, short-term tests, metabolism, and structural/activity relationships.

Stanford Research Institute
Menlo Park, California
An Automated Procedure for Assessing Possible Carcinogenic Activity of Chemicals Prior to Testing
Prepared for National Cancer Institute, Bethesda, Maryland
Contracts: NO1-CP-33285 NIH-NCI-71-2045, 1975

This report discusses the systematic application of information regarding the carcinogenicity of chemicals to the prediction of carcinogenicity activity of untested chemicals. The method focuses on structural relationships between the chemicals being examined and known carcinogens. The development of an activity tree is presented for implementing a procedure for ranking chemicals prior to testing in laboratory animals. The activity tree method classifies a large number of chemicals by asking a series of increasingly more specific questions about their chemical structure. Expert consultants then offer estimates regarding the probability of any chemical in an end point of the tree being carcinogenic and the relative potency of the carcinogenic activity if the chemical proves to be carcinogenic. A level of confidence is attributed to each estimate. Estimates are also made specific to the four routes of administration (i.e., oral, inhalational, dermal, and prenatal) of the compound to the test animal, corresponding to the routes used in the exposure estimates. For the development of this activity tree, six experts offered their considerations on five classes of substances known to contain carcinogens: (1) naturally occurring substances, (2) aliphatic nitrogen-containing compounds, (3) polycyclic aromatic hydrocarbons, (4) aromatic amines, and (5) inorganic compounds. Their reports are summarized and the current activity values for the tree are given. An appendix describes computer implementation of the activity methodology.

Becker, D.S.
IIT Research Institute
Design of a Chemical Hazard Ranking System -- Final Report
Prepared for U.S. Consumer Product Safety Commission
Bethesda, Maryland
Contract No. CPSC-C-77-0068, December 1978

The Consumer Product Safety Commission would like to rank the health hazards of the chemicals in consumer products to enable them to allocate their resources in an appropriate manner. The three main factors of consumer chemical hazard due to consumer products are: (1) toxicity, (2) dose per person, and (3) population exposed. Unfortunately, these factors are not available as standardized statisitics, nor can they be calculated by standardized formulas. Population exposed could be computed from marketing data for each product, but this would be prohibitively expensive. Dose per person should be computable from a product's known characteristics (aerosol, skin contact, frequency of use, etc.), though accepted standardized equations do not exist. Chemical toxic strength factors for carcinogens, mutagens, and teratogens are known for only a few percent of consumer chemicals. No standard method for extrapolating latent toxic strength factors from data on the tested chemicals to the untested ones exists. Typically, these problems have been overcome by having panels of experts rate the three factors based on unstated rules. However, the scope of the problem for consumer chemicals favors a computerized approach based on systematic procedures. First, such a system could efficiently re-rank all chemicals as new data became available. Second, it is less expensive to use automated procedures for this application. Third, it is more precise to make all the decision criteria explicit. This report presents uniform techniques for estimating the toxicity, dose per person, and population exposed factors, and for calculating a hazard score from them. The procedures are sufficiently general that they can be applied, using available data, to all consumer chemicals within an automated system.

Nelson, N.; van Duuren, B; Goldschmidt, B.
Final Report of NSF Workshop Panel to Select Organic Compounds Hazardous to the Environment
National Science Foundation, 1975

A selection process was developed to identify manufactured organic chemicals that may be of special interest because of their effects on environment and/or health. This process is conducted by an advisory panel comprised of members from government, industry, academia, and public interest groups. The selection process was divided into two phases. Phase I identified and ranked 275 compounds in descending order of release rate. The release rate (R) is defined as $R = (P+I)F_D + PF_{PL}$

where: $P$ = the annual U.S. production,
$I$ = the annual imported quantity,
$F_D$ = the fraction of compound which goes to non-intermediate dispersive uses,
and $F_{PL}$ = the fraction of production lost during manufacturing, conversion, and product formulation and that which escapes from the plant site.

Each advisory panel member identified 10 chemicals, regardless of the quantity produced, which they felt merited inclusion on the list. Sixty-two additional chemicals were thus identified and added to the 275 chemicals on the list. Each chemical was independently rated on a scale of 0 (no interest) to 5 (highest interest) by each member. The list was re-ranked using the mean value of the panels' interest and the top 80 chemicals were selected for Phase II evaluation. Phase II evaluation consisted of obtaining data on three factors: (1) production volume, losses to the environment, impurities, etc.; (2) toxicity, covering mammalian, nonmammalian, and environmental effects; and (3) chemical properties, including persistence.

The data for each chemical were reviewed by each panel member and each chemical was discussed by the entire panel. A statement of the panel discussion was prepared for each chemical and the compounds were again rated independently by each panel member for health and environmental effects. The selection process used the combined interests of its diverse membership to rank chemicals for further research.

Brown, S.L.; Chan, F.Y.; Jones, J.L., et al.
Stanford Research Institute, Menlo Park, California
Research Program on Hazard Priority Ranking of Manufactured Chemicals
5 volumes
Prepared for National Science Foundation
Washington, D.C.
NTIS #PB-263 161/2ST; #PB-263 162/0ST; #PB-263 163/8ST; #PB-263 164/6ST; #PB-263 165/3ST, April 1975

This research effort by SRI was divided into two phases. In Phase I, the universe of manufactured organic chemicals was reduced to 250 chemicals according to the highest calculated values for the release rates for these chemicals. Data on relevant physical and chemical properties for these chemicals were presented to the Advisory Panel during its meeting in Menlo Park, California, on August 26-27, 1974. From this list of 250 chemicals and from a list of 41 chemicals designated by the Advisory Panel as "Most Wanted Chemicals," the members of the Advisory Panel selected 80 chemicals for Phase II study as the chemicals with the greatest potential for environmental effects. In Phase II of this two-phase effort, 80 chemicals having the greatest potential for environmental effects were studied. Information was collected on the extent of the environmental exposure to these chemicals (during manufacture and use) and on the possible environmental effects of this exposure (chemical, physical, and biological properties; persistence; and toxicity). A questionnaire survey of industry was conducted to determine the amount and types of losses in the manufacturing plants. Information from this survey is tabulated. The following five summary reports are submitted for each of the 80 chemicals: (1) a flow diagram showing industrial data on the amounts used for various applications; (2) a one-page assessment of the data gathered on toxicology and environmental persistence; (3) a computer printout of a tabular summary of the important data gathered; and (4) copies of the 25 most pertinent abstracts found in the area of toxicology. The report is divided into five volumes.

The first volume contains chemicals 1-20: Tetrakis(hydroxymethyl)phosphonium chloride; Benzo(a)pyrene (BAP); Tetraethyl lead; Vinyl chloride; Hexachlorobenzene; o-Cresol; Ethylbenzene; Nonylphenol, ethoxylated (9 moles of ethylene oxide); Hexachlorobutadiene; Vinylidene chloride; Toluene; Ethylene dibromide; Tris(2,3-dibromopropyl) phosphate; Ethylene dichloride; Trichloroethylene; 1,1,1,-Trichloroethane; Carbon tetrachloride; Chlorinated paraffins (35-64% chlorine); Perchloroethylene; and Dichlorodifluoromethane.

The second volume contains chemicals 21-40: Benzene (chemical uses); Silicone fluids; Nitrobenzene; Toluenediisocyanate (TDI); Xylenes (mixed total); Aniline; Dimethyl terephthalate; Trichlorofluoromethane; p-Dichlorobenzene; Tetrabromoethane; Methylenebis(2-chloroaniline); Polyhalogenated biphenyls (Aroclor 1254); Tricresyl phosphate; Fluorescent brightening agents (no. 23); Polyvinyl chloride; Methylene chloride; Dichloropropene, Dichloropropane mixture; and Ethyl chloride.

The third volume contains chemicals 41-60: (Ethylenedinitrilo)tetraacetic acid, tetrasodium salt; Benzidine; Zinc di(butylhexyl) phosphorodithioate; N-(Dimethylpentyl)-N-phenyl-p-phenylenediamine; Vinyltoluene; Methyl bromide; Mercaptobenzothiazole; Chloroform; Acetontrile; Di(ethylhexyl) phthalate; Vat Blue Dye no. 6 (Dichloroindanthrone); Di(ethylhexyl) adipate; Dimethylamine; Dichlorobenzidine; Hexamethylenetetramine; Acyclic xanthic acid salts (Sodium isopropylxanthate-Dow Z-11); Sulfolane-p-nonylphenyl manganese phosphite; Nitrilotriacetic acid (trisodium salt); and Diarylarylenediamines (mixed) (Wingstay 100).

The fourth volume contains chemicals 61-79: Polyacrylonitrile (fibers); Naphthalene; N,N-Dimethyldodecylamine oxide; Chloroprene; Formaldehyde (37% by weight); Bis(hydrogenated tallow alkyl)dimethylammonium chloride; Methyl chloride; Dioxane; Ethylene oxide; Allyl chloride; Ethylenimine; Phenol; Tri(chloroethyl)phosphate; Polyethylene glycols (MW 400); Methoxyethanol; Dodecylbenzenesulfonic acid (sodium salt); Bis(chloroethyl) ether; Dodecyl mercaptan; Polyurethane and diisocyanate resins; and Ethylene.

The fifth volume contains a listing of the references for the data collected and general notes describing the data.

Stephenson, M.E.
An Approach to the Identification of Organic Compounds Hazardous to the Environmental and Human Health
National Science Foundation
Ecotoxicol. Environ. Safety, 1:39-48, 1977

Results are presented from a workshop ranking hazardous chemicals and identifying key problem areas for future research. Eighty organic compounds were ranked according to their environmental impact and their hazard to human health. A scatter plot of the 80 compounds indicating their relative ranking in terms of both criteria showed that 10 organohalides required immediate study. Seven major impact or problem areas around which future research could be organized include: (1) natural sources of organic compounds; (2) contribution to biochemical and geochemical pools; (3) effects of transport and translocation of toxic elements and micronutrients; (4) toxic degradation products and formation of secondary pollutants; (5) remote effects; (6) persistence in the absence of other effects; and (7) bioaccumulation. It is also recommended that the environmental impact and human health hazard of the carbon-chlorine bond be studied. Production figures and estimated annual release rates for the 80 compounds are given.

Bechmann, R.B; Carhart, H.W.; Cunningham, W.A.; et al.
System for Evaluation of the Hazards of Bulk Water Transportation of Industrial Chemicals
National Academy of Sciences
Contract No. DOT-CG-41.680-A, 1974

An evaluation scheme, developed for the U.S. Coast Guard, to assess the potential hazard of industrial chemicals transported in bulk by water is presented. Each chemical is rated on a scale of 0 to 4 (which reflects increasing hazard) on nine hazard parameters: (1) fire, (2) contact of liquid with skin and eyes, (3) occasional short-term inhalation of vapors, (4) occasional short-term inhalation of gases, (5) repeated inhalation of gases and vapors, (6) human toxicity due to water pollution, (7) aquatic toxicity due to water pollution, (8) reaction with water, and (9) self-reaction (usually polymerization or decomposition). The human toxicity rating is based on the oral $LD_{50}$ in a suitable mammalian species. The aquatic toxicity rating is based on the 96-hour TLm in adult or juvenile fish from upper levels of the food chain and includes special notations on bioaccumulation, biochemical oxygen demand, and insolubility. An appendix evaluates potential concentration ranges of discharged material into three selected receiving system: (1) rivers, (2) estuaries, and (3) coastal waters.

Brown, S.L.; Cohen, J.M.; Macrae, N.I.; Small, M.J.
SRI International
Setting Priorities for R & D on Army Chemicals--Final Report
U.S. Army Medical Research and Development Command
Fort Detrick, Frederick, MD.
Contract No. DAMD17-75-C-5071; CRESS No. 56, May 1978

The Environmental Protection Research Division of the Army Medical Research and Development Command is charged with developing the database for environmental and occupational health criteria dealing with the manufacture, use, and disposal of chemicals in Army activities. This report presents a method that can assist the Army in allocating resources among candidate research and development studies on the environmental and occupational effects of Army chemicals.

The basis of the method is a mathematical model of the process leading from the initial pollution of air, water, land, or the workplace to the eventual environmental or occupational health effects of the chemicals in question. Both environmental and occupational hazard assessment models consider the chemical discharge source; environmental medium; concentration as determined by transport, transformation, and transfer; population at risk; exposure; and effects. Effects in humans include carcinogenicity, severe chronic toxicity, recoverable chronic toxicity, and acute toxicity. Effects in fish include acute and chronic toxicity. Effects are assigned a relative dollar value to allow comparison among different chemicals. For incomplete or missing data on a chemical, the value is estimated, assigned a default value, or assumed to be unimportant. The model estimates a total hazard value, weighted among human and ecological effects, with a corresponding uncertainty value due to lack of knowledge. The allocation method then compares the reduction in hazard uncertainty expected to be achieved after a research study with the cost of the study, and ranks candidate studies according to the ratio.

Margler, L.W.; Rogozen, M.B.; Ziskind, R.A.; et al.
Science Applications, Incorporated, Los Angeles, California
Rapid Screening and Identification of Airborne Carcinogens of Greatest Concern in California
J. Air Pollut. Control Assoc., 29(11):1153-1157, 1979

The method used by the California Air Resources Board to quickly identify and rank potentially serious airborne carcinogens is described. Eight lists of carcinogens were compared after eliminating chemicals not used in California, pesticides, chemicals unstable in air, or doubtful carcinogens. Further eliminations were made if production or use was under 100,000 pounds per year. The investigators included a few additional compounds. Candidate substances were ranked by additive and multiplicative algorithms and by a panel of experts. For the additive algorithm, the rating of a substance was the sum of the scores of each rating factor multiplied by a weighting factor. For the multiplicative algorithm, the substance rating equaled the product of the rating factors. The six criteria rated were: (1) present use, (2) use trends, (3) emission potential, (4) stability in ambient air, (5) dispersion potential, and (6) evidence of carcinogenicity. Those compounds appearing in the top 11 of at least two lists were selected for further study. The substances selected were arsenic, asbestos, benzene, cadmium, carbon tetrachloride, chloroform, ethylene dibromide, ethylene dichloride, nitrosamines, perchloroethylene, and polychlorinated aromatic hydrocarbons. The authors found this screening approach efficient.

Powers, R.; Bednarz, R.; Hurlburt, G.; Koebbe, J.A.; Kavanagh, T.
Michigan's Critical Materials Register and Chemical Hazard Assessment Program
Michigan Critical Materials Register 1980
Department of Natural Resources Environmental Protection Bureau
Environmental Services Division
Publication Number 4833-5324, 1980

Michigan's Critical Materials Register (CMR) system, developed to protect water quality, is described. A list of suspect chemicals is selected annually by an advisory committee from established priority lists and from chemicals of concern in Michigan. The CMR list includes: inorganics, organics, pesticides, herbicides, fungicides, pharmaceuticals, food additives, and natural materials which may be used or discharged in Michigan. Each chemical is scored for eight factors: (1) acute toxicity; (2) adverse effects such as chronic toxicity, fetotoxicity, embryotoxicity, phytotoxicity, and effects of metabolites and degradation products; (3) persistence; (4) bioaccumulation; (5) carcinogenicity; (6) teratogenicity; (7) hereditary mutagenicity; and (8) esthetics. Factors are weighted such that phytotoxicity, persistence, and esthetics have maximum scores of 3, 4, and 1, respectively, and remaining factors have a maximum score of 7. When the data are insufficient to score a factor, an asterisk is assigned and the factor is scored as data become available. Hazard assessment criteria and rationale are presented for each category. Chemicals with a cumulative score of 7 or greater are included in the register. The hazard ranking system has been modified to incorporate potential hazards from air pollutants. Further review of the CMR list focuses on chemicals with the most number of asterisks and chemicals with cumulative scores of less than 7. Businesses are required to file an annual report on the use and discharge of CMR chemicals. The authors note three problems in the assessment program: (1) chemicals lacking sufficient data are not included on the list, (2) lack of adequate chemical composition data on commercial products causes difficulty in identifying products which may contain toxic substances, and (3) many chemicals which may not be used in Michigan are included on the CMR list because Michigan laws do not require reporting of inventory data prior to chemical manufacture and use.

United Nations Environmental Programme
Initial Report on the Priority Pollutants Project
Nairobi, October 1978

Results are presented from the initial phase of the priority pollutants project. The objectives include: compiling a list of hazardous chemicals which have been given priority consideration by governments and other organizations, proposing a systematic process for selecting priority pollutants with emphasis given to the needs of developing countries, and identifying several lists of chemicals or categories for further United Nations Environmental Programme (UNEP) attention. Section 2 includes a compilation of approximately 230 selected substances of concern to various national and international institutions. Section 3 discusses the general problems associated with identifying and ranking environmental hazards. It includes a discussion of the distinguishing features between developed and developing areas which give rise to different sets of priorities for environmental pollution. This section concludes by outlining the selection criteria to be used in a ranking system for both developed and developing areas. Criteria include exposure, carcinogenicity, mutagenicity, teratogenicity, acute toxicity, other health effects, the influence of nutrition and infectious disease on toxicity, persistence and bioaccumulation, and environmental agents. The method uses expert opinion, information on structure-activity relationships, and production and environmental exposure data in a multistage screening process where a relatively large number of substances are considered initially. In subsequent steps, a smaller subset is selected for collection of more data and more thorough review. Section 5 suggests several categories of hazardous pollutants which may be of interest to the UNEP. For each area, an interim list of priority pollutants is proposed.

Brown, S.L.; Cofer, R.L.; Eger, T.; Liu, D.H.W.; Mabey, W.R.; Tus'e, D.
SRI International
A Ranking Algorithm for EEC Water Pollutants--Final Report
Contract No. ENV/223/74-EN: CRESS Report No. 136, September 1980

This report describes an algorithm used to rank 1,500 possible European Economic Community (EEC) water pollutants for prioritization of regulatory action on discharge limitations. Pollutants such as persistent synthetics, mercury, or cadmium compounds already under EEC regulation, compounds produced or used in the EEC in amounts less than 100 metric tons per year, or compounds which could not be identified were eliminated from the list. The remaining 426 pollutants were then ranked by a "screening algorithm" based on production, environmental half-life, and acute toxicity to aquatic organisms and mammals. The top 130 compounds were then ranked using a "complete algorithm" which incorporated information on: sources (amount produced or consumed in EEC and estimated fraction used as an intermediate); discharges (industrial, agricultural, domestic, commercial, water treatment, or unknown); persistence; bioconcentration partition coefficient; acute aquatic effect level ($LC_{50}$); chronic aquatic effect level (TC low); acute mammalian effect level ($LD_{50}$); chronic mammalian effect level (TD low); and chronic mammalian effect reported (carcinogenicity, mutagenicity, or teratogenicity). Each factor was labeled as to whether it was based on reported data or analogy to other compounds and each factor except discharge was scored for reliability. The authors recommend that priority regulatory attention be given to top ranked pollutants with good reliability indexes and that additional data be collected on pollutants with low reliability indexes before taking regulatory action.

Gori, G.B.
Ranking of Environmental Contaminants for Bioassay Priority
International Agency for Research on Cancer, ISS No. 16:99-111. 1977

A ranking index was developed to classify chemicals by their potential hazard and to indicate which chemicals need to be examined first for their carcinogenic properties. The index is based on a quantitative evaluation of their prevalence and distribution in the environment, intake in man, and similarity to known carcinogens. Two major indicators used to determine carcinogenic potential are (1) exposure and intake conditions, and (2) suspicion of activity. Exposure and intake conditions were formulated by analyzing the number of persons exposed and the number of estimated annual intakes per person in each subpopulation. The second indicator, suspicion of activity, was formulated from the probability that the chemical was carcinogenic for each intake route and the estimated relative potency of the chemical for each intake route. Possible contamination from manufacturing processes can affect exposure to a compound and tracing techniques are used to identify sources of contaminants. Forward tracing involves analyzing raw materials of a chemical up to the intake or use by man and identifying contaminants. Backward tracing starts by analyzing an environmental situation and proceeding back to the cause of contamination. Forward tracing examines chemicals with significant production while backward tracing examines compounds with high user exposure. Another method used to aid in confirming suspicion of a chemical as a carcinogen is the chemical structure. Carcinogenic probability and potency estimates for known compounds are determined by an expert panel and ranked into a structure tree. New compounds are compared to the structure tree and, for each intake route, the carcinogenic activity is estimated based on the carcinogenic probability times the estimated carcinogenic potency. With the information incorporated into a single ranking index, any new compound structure may be compared and assigned an index of suspicion. Further development of the system could lead to identifying the carcinogenic hazard of chemicals before they are produced.

Van Netten, C.
Simon Fraser University, Burnaby, British Columbia, Canada
Critical Review of Strategies Aimed at Identifying Chemicals Hazardous to Human Health and the Environment
Prepared for Department of National Health and Welfare, Ottawa, Canada, March 8, 1978

Criteria are presented for evaluating the effectiveness of existing chemical screening strategies. Environmental criteria include production and release, distribution in the atmosphere, degradation, bioaccumulation, and toxicity, as well as synergistic and antagonistic effects within the environment. Human health criteria include exposure of the total population or specific groups, distribution of the substance within the body, accumulation and excretion, general toxicity, mutagenicity, teratogenicity, carcinogenicity, and possible synergistic and antagonistic effects in humans. Decision-making criteria are used to evaluate whether the recommendations made by the different screening procedures allow easy access to information so that specific decisions can be made. Six screening methods are then assessed by these criteria. The author suggests that an optimum combination of these methods could be derived which would reject a maximum number of chemicals at a minimum cost.

Astill, B.D.; Lockhart, H.B., Jr.; Moses, J.B.; et al.
Eastman Kodak Company, Rochester, New York
Sequential Testing for Chemical Risk Assessment
Presented at the Second International Congress on Toxicology
Brussels, Belgium, July 6-11, 1980

A method of quantitatively evaluating environmental and health hazards are presented. Four categories of effects were established: (1) the magnitude of environmental exposure (ME), (2) the magnitude of human exposure (MH), (3) the effects on human health of an exposure (H), and (4) the effects on the environment of an exposure (E). The criteria for MH are production per year, number of people exposed, duration of exposure, and number of groups exposed. The criteria for ME are amount discharged per year, number of discharge sites, number of discharges per year, and half-life in the environment. Criteria for H are the oral $LD_{50}$ in rats, reversibility of immediate effects, and reversibility of prolonged effects. Criteria for E are the 5-hour median inhibitory concentration on waste water treatment microorganisms, the median lethal concentration on fish, and the octanol-water partition coefficient as a measure of bioconcentration potential. Each criterion is given a maximum, median and minimum range and these are ranked 1, 2, or 3, respectively. The cumulative health or environmental score for a compound is evaluated so that scores of 9 or less, 10 to 13, 14 to 17, or 18 or more suggest testing levels I, II, III, or IV, respectively. Level I testing includes physical and chemical properties, acute health effects, in vitro mutagenesis, and acute environmental tests. Level II includes 2-week feeding or inhalation tests, skin painting tests, additional mutagenesis tests, activated sludge effects, photodegradation, biodegradation, effects on plant growth and germination, and partition coefficients. Level III includes 90-day feeding or inhalation, fertility tests, teratology, half-life and metabolites in rodents, nitrification inhibition, algal toxicity, 14- to 21-day biodegradation, simulated fate study, larval fish studies, and bioconcentration factor. Level IV includes 2-year feeding studies, 3-generation reproduction studies, teratology, pharmacokinetics, biodegradation products, soil interaction, and long-term aquatic studies. If testing is conducted, the results may then be entered into the scoring and the total score reassessed. The authors conclude that this screening protocol is both cost and time effective, as over 500 chemicals have been tested in 2 years.

Nees, P.O.
Hooker Chemical Company, Niagara Falls, New York
Assessment of Oncogenic Potential - A Scoring Matrix to Determine Oncogenic Potential Proposed for Application in Risk Assessment
In: Toxic Substances Control, Vol. III - Implementing the Regulatory Program
Miller, M.L., ed., Government Institutes, Incorporated
Washington, D.C. pp. 168-82, 1979

A scoring matrix for oncogenic risk assessment that assigns weighted number values to subjective and objective results of studies is described. Positive lifetime animal studies receive a primary score of 4, which is multiplied by metabolism, route of administration, and quality of study scores. This result is then weighted with a dose level factor and a time until tumor appearance factor. Negative results start with a minus primary score and the time weighting is correlated to survival. Epidemiology studies have a primary score of 10 multiplied by specificity of tumor type, suitability of controls, indirect association, relative risk, mixed exposure, and specificity factors, and added to a detectability of increased cancer incidence factor. The resulting adjusted primary score (AP) is weighted by adding AP times a dose response factor to AP times a consistency of association factors to AP times an exposure level factor. There is also a weighting for repetitive epidemiological studies to compensate for low confidence level in a single study. Negative studies start with a primary score of 6 and have fewer factors. For short-term genetic, microbial, and fluid assays, individual test scores are small, positive or negative, and the only weighting factor is for supportive data. The sum of all the scores is ranked on an index of oncogenic potential that correlates the total score to an appropriate regulatory response. The author concludes that the scoring matrix can be used by people with little experience. An expert review panel would be necessary only if questions arose. The assessment could change with the results of new studies.

Kimerle, R.A.; Gledhill, W.E.; Levinskas, G.J.
Monsanto Co., Environmental Assessment Department, St. Louis, Missouri
Environmental Safety Assessment of New Materials
In: Cairns, J.; Dickson, K.L.; Maki, A.W.; Eds.
American Society for Testing Materials STP No. 657:132-146, 1978

A procedure is presented for evaluating the hazard to aquatic organisms of new materials prior to their commercialization. The procedure uses environmental fate and aquatic organism toxicity data in the sequential phases of screening, predicting, confirming, and monitoring to reach a decision either to continue the toxicity testing, terminate the project because of unacceptable risk, or cease testing because of an acceptable risk. The screening phase involves short-term acute tests, while the predictive phase involves short- and long-term laboratory studies. In the confirmation phase, environmental field studies are designed to answer critical questions of environmental safety. In the monitoring phase, field studies under actual use conditions after commercialization are conducted to confirm the ultimate safety of the material. The types of tests in each phase and the criteria that determine which specific tests are needed are presented. The criteria for evaluating whether or not a hazard exists also are discussed.

Booz Allen Applied Research, Inc.
A Study of Hazardous Waste Materials. Hazardous Effects and Disposal Methods
Vol. 1, 1973

A system is described for rating hazardous materials. One rating equation is based on known data and a second rating equation is used for assessing compounds with unknown data. The first equation is HR = TER x HER

where: HR is the hazard rating,
TER is the total effects rating,
and HER is the hazard extent rating.

TER is the sum of values assigned for air, water, and soil contaminant hazards on human populations; effects from flame, explosion, or reaction of the material; and toxic effects on ecological populations. Toxic effects include acute and chronic $LC_{50}$ and TLV for air and water, and effects of contact exposure for soil. Each factor can be weighted to reflect importance. The score for each of the factors may be U (unknown), 1 (minimal hazard), 2 (slight to moderate hazard), or 3 (severe hazard). HER is the sum of production and consumer distribution scores. Production scores are based on the amount produced per year and may be U (unknown), 1 (low), 1.25 (moderate), or 1.5 (large). Consumer distribution scores may be 0 (limited), 0.25 (moderate), or 0.5 (wide). Criteria for scoring TER and HER are presented.

The second equation is MPHR = (3U + TER) x HER

where: MPHR is the maximum potential hazard rating,
and 3U = a rating of 3 to each unknown to produce a conservative hazard rating.

Ratings are given for many hazardous materials used as warfare agents.

Jones, C.J.
The Ranking of Hazardous Materials by Means of Hazard Indices
J. Hazard. Mater., 2:363-389, 1978

Several indexing models for use in landfill management, transport of dangerous goods, environmental quality assessment, and other areas are reviewed. Suggestions are then presented for developing a hazard index for evaluating waste management options. The procedure involves listing the materials or wastes of interest and the management or disposal options to be considered. The properties of the materials or wastes which are relevant to the evaluation process are obtained from the existing literature or from laboratory measurements. A combination model appropriate to the management situation must then be constructed. The author recommends the additive utility model, but notes that other models may be more appropriate in certain cases. The normalized indexes for each material and the relative utility range for each property are derived from the data and the overall index is calculated using the combination model. The overall indexes must reflect the actual properties of the material in combination with the relative importance attributed to each property by the weighting factor. The author observes that if the combination model is mathematically sound, the use of an indexing and combination model allows versatility in quantifying value judgements about aspects of a given material's environmental behavior.

Cramer, G.M.; Ford, R.A.; Hall, R.L.
Estimation of Toxic Hazard -- A Decision Tree Approach
Food Cosmet. Toxicol., 16(3):255-276, 1978

A procedure using 33 criteria for establishing toxic hazard is presented as a decision tree organized into branches dealing with major chemical classifications. The procedure is intended for use with all ingested, structurally-defined organic and metallo-organic substances. The criteria are based on features of chemical structure, occurrence in body tissues and fluids, and natural occurrence in food. The logic of the tree rests heavily on known data on metabolism and toxicity. The classification according to presumptive toxicity can be combined with knowledge of human intake to provide a protection index for each substance. The index can be used to establish priorities and define tentatively the extent of appropriate testing. It is noted that the procedure has been applied to a large number of pesticides, drugs, food additives, and industrial and environmental chemicals of known biological properties. Because the procedure has not yet resulted in any underestimation of toxicity, it is seen as a practical means for discriminating effectively among different levels of probable hazard.

Cairns, J.; Dickson, K.L., Maki, A.W.
Estimating the Hazard of Chemical Substances to Aquatic Life
Hydrobiologia, 64(2):157-166, 1979

A conceptual framework for conducting a hazard assessment is presented. Various toxicity tests and procedures for evaluating hazards to aquatic life are compared, and the decision criteria used in these procedures are discussed. The use of safety factors or "uncertainty factors" is discussed as a central concept in a sequential testing approach in which estimates of expected chemical concentrations in the environment and their effects can be made with an increasing degree of accuracy. The state of the art of assessing hazards from chemicals to aquatic life is reviewed; safety, hazard, and risk concepts involved in such assessments also are discussed. Particular attention is given to hazard assessment procedures developed by the American Society for Testing Materials, the American Institute of Biological Sciences, and Monsanto.

Ingraham, T.R.; Zechel, E.M.
Selection of Candidate Substances for Control in an Environmental Regulatory Agency
J. Air Pollut. Control Assoc., 29(1):38-42, 1979

A quantitative decision-making process based on the serial application of three models and incorporating measured data and subjective judgment is presented for selecting environmental regulation candidate substances. The first model defines the severity of a pollution problem. Values assigned for damage to an individual organism, concentration of the pollutant, percentage retention of the pollutant, duration of exposure, hazard to the organism, and the total population of organisms are multiplied to attain the total damage index. The second model defines the social, economic, and political impact of regulation. Values assigned on a scale of -5 to +5 for nine factors: (1) public health protection; (2) employment and income stability; (3) lifestyle changes; (4) creation of income disparity; (5) alterations in market structures; (6) changes in regional, provincial, or national balance of payments; (7) public acceptance; (8) effects on territorial sovereignty; and (9) contribution to inflation, are totaled to determine impact. The third model assesses the current technological capability for implementing a potential regulation. Values assigned to reliability, efficiency, general applicability, dollar and manpower resources, and development in a given period of time are multiplied to attain the magnitude of the technological capability. Illustrative cases are given for each model.

Keith, L.H.; Telliard, W.A.
Priority Pollutants. I. A Perspective View
Environ. Sci. Technol., 13(4):416-423, 1979

The historical origins of the EPA Priority Pollutants and the development of the Priority (Water) Pollutants Protocol are related. Events are traced beginning with the court decision in 1978 that resulted in adoption of the EPA Consent Decree to control the levels of pollutants in industrial wastewater discharges. Components of the decree are reviewed, including formation of the Toxic Pollutant List to aid in the classification of harmful substances. It is noted that, since the decree lacked allowance for time in solving analytical problems in testing for these substances in wastewaters, the EPA adopted four criteria to prioritize and select representative compounds from each group. (1) All compounds specifically named on the Toxic Pollutant List were automatically included. (The availability of chemical standards for verification and quantification was considered mandatory. (2) Compounds not found on the list should be tested if they accounted for 5% or more of the total known listing for the class of compounds. (3) All chemical production data should be reviewed, where available. (4) Other sources were examined to determine if the compound was a recognized water pollutant. Next, the screening, verification, and monitoring strategy developed by the EPA for testing water for pollutants is presented. Unresolved problems in the screening stage are discussed, along with automated software programs being adopted to speed up the analysis process. Future plans and first drafts for implementation of the monitoring phase are considered, and a list of the 129 compounds on the Toxic Pollutant List is included.

Langner, R.R.; Norwood, S.K.; Socha, G.E.; Hoyle, H.R.
Two Methods for Establishing Industrial Hygiene Priorities
Am. Ind. Hyg. Assoc. J., 40(12):1039-1045, 1979

Two approaches, health team rating and calculation rating, are described for determining the health hazard of industrial chemicals and establishing industrial hygiene priorities. In health team hazard rating, a team composed of an industrial hygienist, physician, toxicologist, safety engineer, and process engineer rates the degree of exposure and consequences of overexposure to a chemical for each job classification in a facility. Degree of exposure ratings are no contact, minor contact, occasional daily contact, and gross contact likely. The assessments of the consequences of overexposure are based on acute toxicity, chronic toxicity, and available data on eye, skin, inhalation, and ingestion exposures. The health team then ranks each chemical for each job classification on a scale of 1 to 5. Class 1 chemicals have a significant probability of a serious overexposure and require immediate investigation. Class 2 chemicals have a possibility of overexposure, but with less severe consequences than Class 1, and should be monitored after investigating Class 1. Class 3 chemicals have satisfactorily controlled exposure and regular monitoring is recommended. Class 4 chemicals have only a remote possibility of overexposure with serious consequences and require only confirmatory monitoring. Class 5 chemicals pose no health hazard and require no monitoring.

Calculated ratings can be used to assess the health hazard of numerous chemicals under varying conditions and use. A formula is presented for calculating hazard due to inhalation of gases and vapors. Parameters included in the formula are: degree of exposure, consequences of overexposure, atmospheric boiling point, and the maximum airborne workplace concentration to which a chemical should be controlled to prevent significant adverse health effects to an employee. Degree of exposure is rated on a scale of 1 to 5, including the four categories described previously plus a penalty factor of 1 that is added when the process is operated at greater than 5 atmospheres of pressure. Consequences of overexposure are rated on a scale of 1 to 4 according to the seriousness of employee health effects. The calculated hazard rating corresponds to five subsequent action steps similar to those previously described. The authors note that both approaches are based on hazard rather than toxicity, thereby allowing appropriate establishment of hygiene priorities. They further note that the calculated health hazard may be a more useful method in determining regulatory action and is adaptable for computer use for broad-based studies.

Branson, D.R.
Prioritization of Chemicals According to the Degree of Hazard in the Aquatic Environment
Environ. Health Perspect., 34:133-138, 1980

An aquatic hazard assessment technique is proposed for prioritizing chemicals. Aquatic hazard is defined as the margin between the no observable adverse effect concentration (NOAEC) and the ambient exposure concentration. In fish, the safety margin is the NOAEC in chronic or sensitive life-stage tests divided by the ambient exposure concentration in water. In fish eaters, the safety margin is the acceptable daily intake of residues in fish divided by the ambient concentration in fish. Ambient exposure concentrations may be measured directly or predicted from a nomogram based on the ambient concentration in fish and the ratio of relative dissipation and bioconcentration potential. A chemical with a safety margin of 5 or higher is classified as a priority chemical.

Kornreich, M.R.; Nisbet, I; Fensterheim, R.; et al.
Clement Associates, Inc.
Priority Setting of Toxic Substances for Guiding Monitoring Programs
Contract No. OTA-C-78-372, 1980

Thirty-two previously existing priority lists for monitoring, testing, or regulating chemicals are reviewed. The values of the lists are discussed and a new priority system for monitoring potentially toxic chemicals in food is proposed. A master list of priority chemicals was comprised from established priority lists as well as chemicals recommended for inclusion by an advisory panel. Through panel decision, select classes of chemicals were removed from the master list to shorten the list and concentrate on food contaminants of greatest concern. The chemical classes removed from the list were pesticides, drugs, intentional food additives, chemicals not in commercial production, and chemicals with limited occurrence in the environment. The remaining organic chemicals on the list were grouped into class categories, e.g., chlorinated benzenes, cresols, xylenes, etc., to further reduce the list. All compounds of each metallic element were considered as a single group and all forms of asbestos were grouped together. The problems associated with such grouping and evaluating representative chemicals from each group are discussed. The chemicals were evaluated on exposure and biological factors. Exposure factors included data on bioaccumulation potential, environmental persistence, occurrence in water, production, use pattern, occurrence in foods, potential for post-sale contamination, and volatility of organic chemicals. Biological factors included acute toxicity, carcinogenicity, mutagenicity, teratogenicity, other toxic effects, and health effects attributed to food contamination. Weights were assigned for each factor and a total score was computed. Objective criteria were used to score each factor when possible (e.g., oral $LD_{50}$ for acute toxicity), but, when necessary, subjective judgment from the expert panel supplemented the objective data. Problems associated with ranking systems such as this one, e.g., unknown data, are discussed. A separate ranking system is proposed for radionuclides.

Oller, W.L.; Cairns, T.; Bowman, M.C.; Fishbein, L.
A Toxicological Risk Assessment Procedure: A Proposal for a Surveillance Index for Hazardous Chemicals
Arch. Environ. Contam. Toxicol., 9(4):483-490, 1980

The Surveillance Index (SI) is a quantitative method to rank the potential risk of suspect food residues for prioritization in food residue monitoring programs. The SI is equal to the sum of the toxicity factor (TF), environmental factor (EF), and biosafety factor (BSF) (SI = TF + EF + BSF). The TF is equal to the kilotons of a compound released annually into the environment (KT) multiplied by the relative toxicity ratio (RTR) of the oral $LD_{50}$ in rats of dieldrin to the $LD_{50}$ of the suspect compound. The EF is equal to the effective half-life (1/2E), which is calculated from the physical half-life and biological half-life, multiplied by the sum of crop values (CV). Values are assigned to crops in which residues are likely to occur based on preparation required for the commodity prior to consumption, principal consumers, and the time interval between crop harvest and consumption. Values are high for nonprocessed crops such as vegetables and fruit, and low for fully processed crops. The BSF is determined by values for the propensity to biomagnify (PB), reactive sites in man, population at risk (PAR), and the no observable effect level (NOEL) according to the equation BSF = PB x S x PAR/NOEL. To evaluate banned compounds, naturally occurring compounds, and contaminants, a modified SI (MSI) is calculated according to the equation MSI = (RTR x EF) + BSF. The SI is determined for several known food residues and found to be valid. The authors note that the effect of nontoxic changes, such as usage/production, on the SI is minimal compared to the impact of changes in toxicity data.

McErlean, A.J.; Duke, T.W.
On the Use of Indices in Aquatic Toxicological Hazard Assessment
Regulatory Toxicol. Pharmacol., 1(3-4):344-354, 1981

An environmental index to assess the potential aquatic toxicity of chemicals is described. For each environmental factor, the chemical is ranked on a subindex scale ranging from 0 to 100. The range for each subindex scale is determined from the highest and lowest values of its known compounds and converted to a 0 to 100 scale. Each subindex score is raised to a power and multipled together to calculate the total index value. The sum of the subindex exponents equals 1 to ensure a range of 0 to 100 for the total index. Variable weighting of the subindex exponents can be used to reflect relative importance of individual factors. The calculated total index value of the chemical can be compared to total index values for known compounds in order to rank relative aquatic hazard. An example is presented using three factors: (1) an invertebrate $LC_{50}$ toxicity test, (2) a vertebrate $LC_{50}$ toxicity test, and (3) the octanol-water partition coefficient. The authors note that the advantages of this technique include utilization of existing data and rapid identification of hazardous chemicals.

Squire, R.A.
Ranking Animal Carcinogens: A Proposed Regulatory Approach
Science, 214(4523):877-880, 1981

A method is proposed for ranking identified animal carcinogens into five classes with varying regulatory options. It is assumed that the carcinogens have been identified by testing at multiple doses and in at least two species. Carcinogens are scored for six factors: (1) number of different species affected, (2) number of histogenetically different types of neoplasms in one or more species, (3) spontaneous incidence in appropriate control groups of neoplasms induced in treated groups, (4) dose-response relationships, (5) malignancy of induced neoplasms, and (6) genotoxicity as measured in a battery of tests. Possible total scores range from 13 to 100. Class I carcinogens would have total scores of 86 to 100 and the regulatory options would be restriction or banning. Class V carcinogens would have total scores less than 41 and there would be several regulatory options including no action, limited use, labeling requirements, and/or public education programs. Regulatory options on Class II, III, and IV chemicals would fall between those for Class I and Class V chemicals.

Schmidt-Bleek, F.; Haberland, W.; Klein. A.W.; Caroli, S.
Steps Towards Environmental Hazard Assessment of New Chemicals (Including a Hazard Ranking Scheme. Based Upon Directive 79/831/EEC)
Chemosphere, 11(4):383-415, 1982

A scheme is presented for environmental hazard ranking and hazard assessment of chemicals prior to marketing. Appropriate parameters of air, water, and soil/sediment are scored and used to calculate effect and exposure in each media. Effect parameters include: acute fish toxicity, acute Daphnia toxicity, oral or inhalation 28-day mammalian toxicity, mutagenicity screening, and skin sensitivity. Exposure parameters include use patterns, bioaccumulation potential, environmental compartmentalization, and persistence. Effect and exposure point allocations are presented. Inherent risk for each medium is determined by multiplying effect and exposure and then is standardized. Based on the inherent risk scores as compared to known chemicals, chemicals are then assigned to one of three categories: (1) white, no immediate regulatory interest; (2) gray, keep under consideration; and (3) black, immediate further testing required. A case illustration is presented for DDT.

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Persons interested in the control of toxic chemicals have examined and are examining methods to select chemicals of concern from the universe of chemical substances. Chemical selection refers to such activities as priority-setting, ranking, indexing, and sorting. These efforts have included the development of various systematic selection methods, such as scoring systems. This annotated bibliography is intended to provide brief summaries of a variety of chemical selection methods.

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