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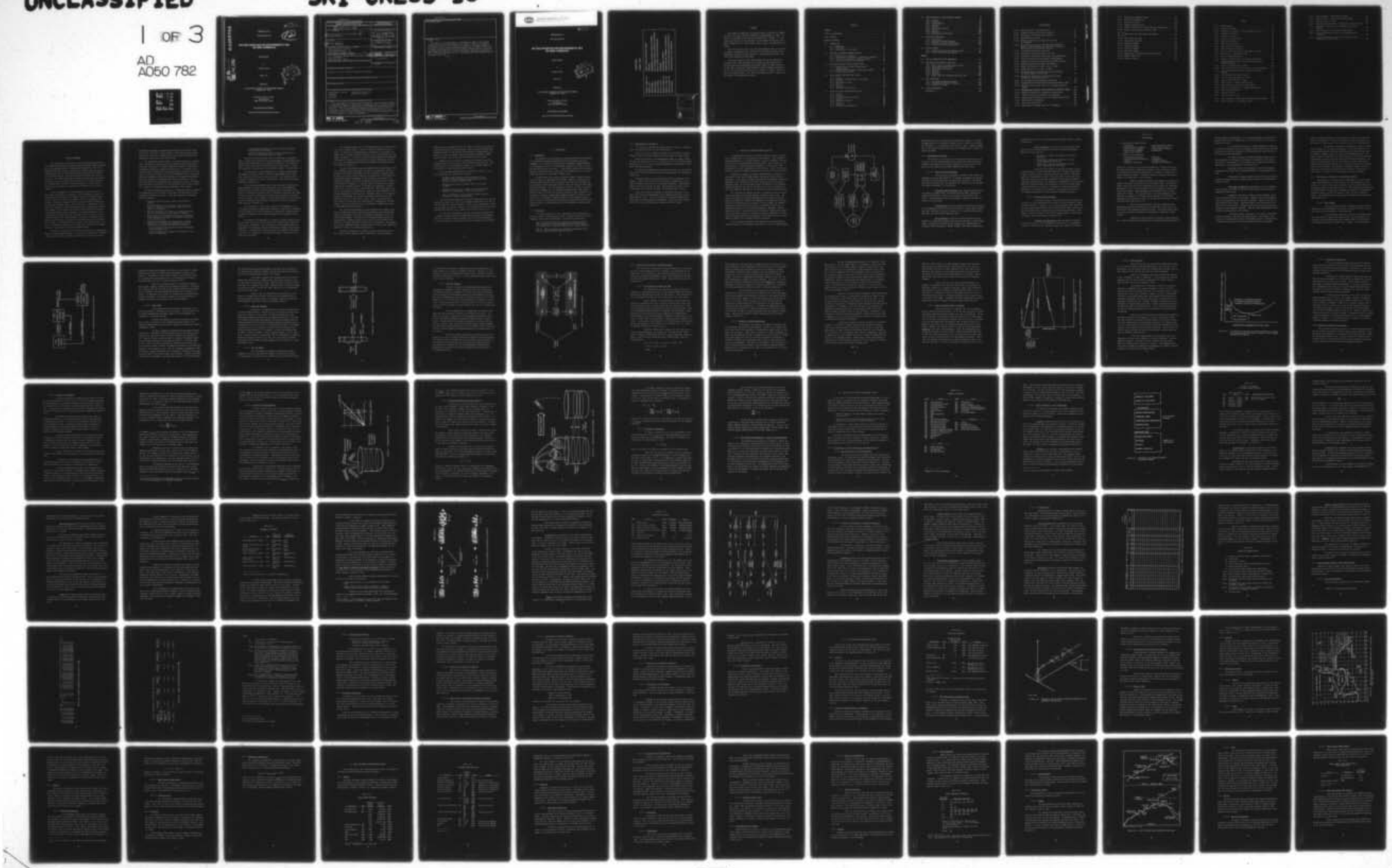

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SRI Project EGU-4479

SETTING PRIORITIES FOR ENVIRONMENTAL R&D ON ARMY CHEMICALS

ANNUAL REPORT

by

Stephen L. Brown

January 1977

Supported by

U.S. ARMY MEDICAL RESEARCH AND DEVELOPMENT COMMAND
Washington, D.C. 20314

Contract No. DAMD17-75-C-5071
SRI International
Menlo Park, California 94025

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The Environmental Protection Research Division of the Army Medical Research and Development Command is charged with recommending criteria for environmental standards dealing with the manufacture, use, and disposal of chemicals in Army activities. This report presents a methodology that can assist the Army in allocating resources among candidate research and development studies on the environmental effects of Army chemicals, in a cost-effective manner with respect to the development of criteria for standards.

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The basis of the methodology is a mathematical model of the process leading from the initial pollution of air, water, or land to the eventual environmental effects of the chemicals in question. The model estimates a total hazard value, weighted among human and ecological effects, with a corresponding uncertainty due to lack of knowledge. The allocation methodology 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.

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PREFACE

This report is submitted as an annual report on Contract No. DAMD17-75-C-5071, and covers all work completed through December 31, 1976. As such, it is complete within itself and stands alone. However, it is intended that the bulk of this document will eventually become part (probably as Appendix A) of a final project report, and it is organized accordingly.

This first annual report covers the environmental phase of a project to develop a methodology for cost-effective allocation of research and development resources on Army chemicals. The second annual report will cover the occupational health phase.

This report would not have been possible without the significant contributions of many SRI experts and consultants (see Frontispiece). We also gratefully acknowledge the technical input and support given us by the staff of the Army's Environmental Protection Research Division at Ft. Detrick, Maryland, especially by Capt. Walter P. Lambert, Mitchell J. Small, and Gareth Pearson. Mr. Small contributed directly to Annex A.B, "Procedures for Preparing Input Data."

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EXECUTIVE SUMMARY

Two complementary methodologies have been developed and tested to assist EPRD in allocating its resources among competing research programs on the environmental hazards of Army chemical pollutants. The first methodology entails a hazard estimating and ranking system consisting of a mathematical model of the pollution process which provides estimates of the relative hazards of different chemicals released from different locations. The second methodology estimates the uncertainty--in each of the hazard values--resulting from uncertainties in the input variables of the hazard model, and then allocates resources to those research studies that most reduce the uncertainty in hazard per unit of cost of research.

A basic assumption of the methodologies is that when little is known about the hazards of a chemical in the environment, one must set very conservative standards (for example, emission or effluent guidelines) in order to be sure of acceptable levels of environmental protection. This basic assumption inevitably leads to higher expenditures on pollution abatement than are really necessary. Consequently, expenditures on research are justified when much can be learned about substantial hazards, since, without the research, these hazards will probably require unnecessarily large investments in pollution abatement. These considerations establish that the principal criteria for selection of a research study are the estimated hazards on which it contributes information, and the degree of reduction in uncertainty that can be achieved by the study. A third criterion is the cost of the study, because a series of inexpensive studies can often reduce more uncertainty in hazards than can a single study costing an equivalent amount.

Hazards are defined in terms of effects predicted by a mathematical model of environmental pollution. An effect can be any adverse biological condition such as cancer in humans, fish kills, or yield loss in crops.

To provide a standard of comparison among effects of different kinds, each effect is assigned a value relative to the others; in the present system, the values are in monetary units, and hazards accordingly are expressed in equivalent dollar loss per year.

The fundamental hazard estimate is one that applies to a specific effect incurred by a specific group of individuals from a given population type, and caused by a specific chemical released to a specific environmental medium from a specific Army facility. For example, such a "six-subscript" hazard would be the expected dollar per year loss attributable to fish kills (effect) in the fish (population type) in Bluestone Reservoir (population group) from discharge of nitroglycerin (chemical) into water (medium) by the Radford AAP (facility location). The six-subscript hazards can be aggregated in various ways to give, for example, the total hazard attributable to a given pollutant from a given location for all media, all population types and groups, and all effects.

The hazard methodology consists of a mathematical model, procedures for gathering data for variables of the model, and procedures for exercising and interpreting the model. The model contains the following general components:

- Valuation--Assigns relative values to the different effects.
- Effects--Estimates the fraction of a population group that will experience a given effect from a given exposure to a pollutant.
- Exposure--Determines the exposure of a population group given the concentration in the medium of exposure.
- Population-at-risk--Determines the size of a population group (ordinarily the number of individuals) exposed to a given concentration.
- Concentration--Determines the concentration to which populations are exposed from measurement of or basic information on environmental behavior, including:
    - Sources--Estimates the amounts of pollutant discharge to environmental media.
    - Transport--Models the transport of pollutants in air, water, or groundwater.

- Transformation--Estimates the rates at which pollutants are chemically transformed.
- Transfer--Estimates the rates at which pollutants move from one environmental medium to another.

Separate concentration models for air pollutants (a dispersion model), surface water pollutants (a dilution model), and groundwater pollutants (a diffusion model) are currently implemented. The groundwater model includes provisions for percolation into surface water. Concentration may also be generated by other models external to the main model.

The main model has been implemented as a computer program HERS. The program is unusual in that it features standardized input formats that allow data to be input in almost any order. The program is also relatively insensitive to errors or omissions of data, and gives copious diagnostic information.

The allocation methodology builds upon the hazard estimating and ranking system by estimating the uncertainties in selected aggregate hazards before and after a proposed research study. Uncertainty is defined in the Bayesian subjective sense, in which the scientists who supply values for the input variables also express their subjective evaluation of their accuracy. Most commonly, an "uncertainty factor," U, is selected which sets subjective 95% confidence limits $\hat{x}/U$ and $\hat{x}U$ on a variable x that has a best estimate of $\hat{x}$.

The uncertainties in the input variables are propagated to the six-subscript hazards and aggregations thereof by a Monte Carlo technique, in which samples of the input variables are combined by the hazard model into hazard estimates, and the sample hazards are then analyzed statistically.

The hazards to be aggregated to evaluate a specific research study are all those that contain one or more of the variables about which the study gathers information. The uncertainties in the input variables are propagated to the aggregate hazard for both the pre-study and post-study situations. The Monte Carlo technique results in a sample of hazards for each of the two situations, and standard deviations of hazard are calculated for each sample.

The difference between the two standard deviations, divided by the cost of the research study, is used as an index of preference for the study. If criteria for nonquantifiable considerations are lacking, the studies with the highest indexes should be selected for funding until the budget is exhausted. In practice, there are many important considerations that cannot be treated in the objective allocation methodology, and the results of the methodology should provide guidance to program selection but should not dominate it.

The research programs conducted by EPRD include toxicological studies in mammals, aquatic organisms, and plants; environmental chemistry related to persistence and movement in the environment; chemical characterization of waste streams; sampling of concentrations of pollutants in environmental media; measurement of the quantities of pollutants discharged; development of analytic techniques; and field surveys of aquatic and terrestrial ecosystems. A research study is defined as any program conducted on a specific subject, for example, the sampling of cyclohexanone in air in the vicinity of the Holston AAP. Each study consists of one or more projects to determine the values of specific variables in the hazard estimating and ranking system. Candidate studies for the current allocation methodology are chosen by excluding studies that have been completed, started, or definitely planned; studies that cannot begin until others are completed; and studies that are inappropriate for other reasons, such as the existence of an environmental standard that cannot be influenced by further research.

The allocation methodology has been implemented for computer operation by adding Monte Carlo uncertainty propagation, hazard-uncertainty reduction, and index of preference calculation capabilities in an allocation program AMRDCP. The inputs to the expanded program include the specification of research studies, their costs, and the residual uncertainties in variables expected as an outcome of the studies. The program as currently implemented cannot evaluate research studies with complicated patterns of effects on variable uncertainties.

The hazard estimating and ranking system has been exercised on a set of about 30 Army chemicals and 5 civilian ones. Hazard estimates ranging from over $400,000 per year for RDX to less than $1 per year for several pollutants have been generated. Other pollutants showing high estimated hazards are TNT and the dinitrotoluenes, nitroglycerin, and chlorates. Civilian chemicals appear to warrant considerably higher hazard estimates, some in the tens of million dollars per year.

Hazards are very often due to human health effects rather than nonhuman effects, but the number of such effects predicted is low. The consideration of the environmental behavior of a pollutant appears to be essential for understanding relative hazards.

The following recommendations are offered with respect to the hazard estimating and ranking system results:

- The HERS program should be used periodically as one element in the surveillance of Army-related pollution problems to suggest abatement needs.
- Additional input data and models should be developed for HERS.
- Expanded research areas for EPRD, such as environmental chemistry or epidemiology, should be considered.
- Some consideration of the system's data needs should be included in research program design.

The allocation methodology is currently being tested with the Army chemical data base (air, water, and groundwater pollutants) and a set of over 200 candidate research studies. Results are too preliminary to make any defendable conclusions. However, it does appear that the very highly desirable programs will have a benefit-cost ratio in excess of 1.0.

The allocation methodology computer model requires improvements to reduce the required number of Monte Carlo simulations to manageable size, and to process research programs that the current algorithms do not evaluate properly even though all input data elements are available.

A.1 INTRODUCTION

A.1.1 Background

One mission of the Environmental Protection Research Division (EPRD), U.S. Army Medical Bioengineering Research and Development Laboratory (USAMBRDL), U.S. Army Medical Research and Development Command (USAMRDC), is to recommend criteria for environmental standards on chemical pollutants generated by Army activities. A substantial research and development program is required before criteria can be recommended that will protect health and welfare at reasonable abatement costs.

The Army deals with a large, increasing number of chemical pollutants at a variety of geographical locations. Research studies directed toward certain chemicals and locations are more useful in learning about and eventually controlling adverse effects than are those for other chemicals and locations. For each pollutant of concern, a number of research studies are caididates for the standard-setting process. Some studies are more useful than others in reducing uncertainty about standards. The selection of the most valuable among competing research studies is often not obvious. Consequently, EPRD requested Stanford Research Institute (SRI) to assist in developing and exercising a systematic method for guiding the process of setting priorities for environmental research on Army chemicals.

A.1.2 Objectives

The overall objective of this investigation was to develop and exercise a method for guiding the process of setting priorities for environmental research on Army chemicals. Two tasks were identified:

> Task I: Develop and exercise a method for ranking Army chemicals according to their environmental hazards, and compare this ranking with a similarly ranked list of civilian chemicals.
>
> Task II: Develop and exercise a method for allocating scarce resources among candidate research projects.

A.1.3 Organization of the Report

This report is organized in several levels of detail so different users can read selectively for their own purposes.

Section A.2 gives a complete overview of the problem of research program selection and SRI's approach to its solution, but omits detail.

Most of the details of the mathematical model for hazard ranking are given in Sections A.3 to A.6. Section A.3 lays out the overall model, and Sections A.4, A.5, and A.6 show the differences in treatment for air, water, and land pollutants.

The allocation methodology is detailed in Section A.7, and initial results for both the hazard and allocation methodologies are discussed in Section A.8.

Supporting material of specialized interest in contained in the annexes. Annex A.A is a listing of references, accompanied by a cross index of mnemonic codes used in the detailed procedures. References are noted in the text by author and date. This technique is used to avoid renumbering when references are added in subsequent annual reports.

Annex A.B describes procedures for preparing input data to the hazard and allocation methodologies and is designed especially for the EPRD scientific staff. Annex A.C describes the computer-assisted data processing for data-processing professionals. Annex A.D gives selected data on the civilian production of chemicals used by the Army.

A.2 OVERVIEW OF RESEARCH PROGRAM SELECTION

To understand the process of research program selection, one must first consider what is to be achieved by the research. Most of EPRD's research programs are in applied research. They are intended to be used as the basis for action-oriented decision making. Some research is conducted merely to understand natural phenomena, in the hope that some discoveries will have additional practical payoffs. This is called basic research, and some of EPRD's resources are set aside for such activities.

Research is valuable for decision making because it reduces the uncertainty of the decision makers about the likely outcome of their decisions. In the case of setting standards for environmental pollutants, research not only establishes with more certainty the levels that are acceptably safe, but also provides a basis for defense of the standards against charges that they are too stringent (too costly to achieve for the safety benefits received) or too lax (allow too many adverse effects).

The rationale for applied research on standards is thus the reduction of uncertainty in decision making, as shown in Figure A.2-1. The person who selects the research programs (makes allocation decisions) needs a rationale for research that depends on the operational decisions that will be influenced by the research. He must examine the research program choices and the existing state of information to arrive at a preferred allocation of the resources (personnel, equipment, contract funds, and so on). He can divide his rationale for research into quantifiable objectives, subject to systematic evaluation procedures, and subjective elements that cannot be expressed in hard scientific form. Both should be used for the ultimate allocation decisions.

The investigations reported here address only the quantifiable, systematic part of the rationale, which leads to a list of ranked program

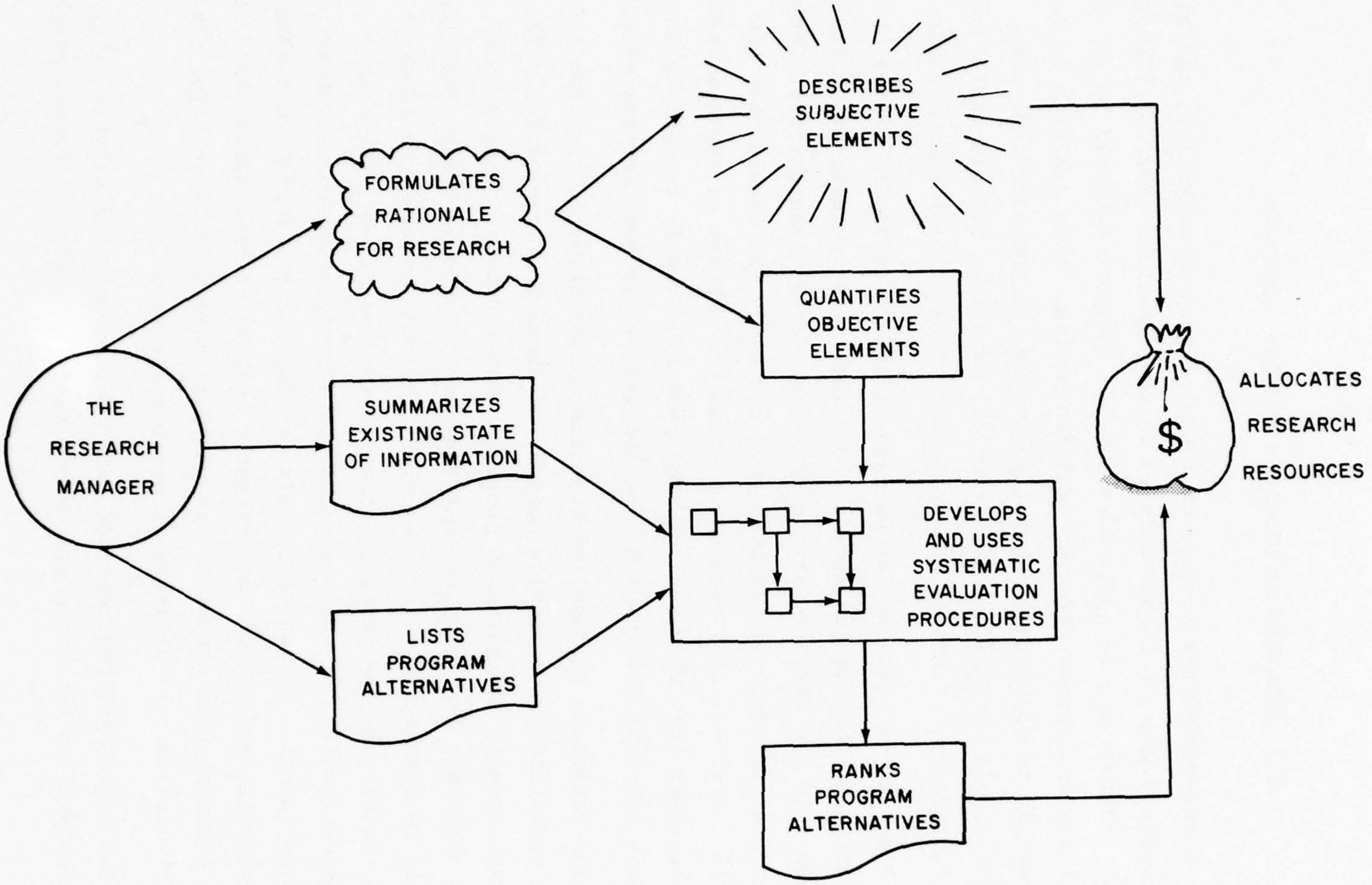

FIGURE A.2-1 RESEARCH PROGRAM SELECTION PROCESS alternatives that can be reordered with subjective criteria. It should be emphasized that a systematic procedure is only a guide in the allocation decisions. It is necessarily too limited to give a complete answer, but it can provide insights that would not be possible with a purely subjective procedure.

A.2.1 EPRD Research Interests

This section is a review of both the Army activities that are of concern to the environmental phase of the project and the EPRD research programs that address the pollution problems of these activities. The section can be skipped by any reader familiar with these facts.

A.2.1.1 Army Activities Considered

The two pollution problems of concern in this report are discharges from munitions plants to the general environment and residual pollution on Army installations from past Army activities. The latter case involves concern about the standards for restoration of an installation before returning it to civilian use.

Munitions Plant Discharges--Army munitions plants, which are usually government-owned, contractor-operated (GOCO), manufacture explosives and primers, and they load and pack these materials into shells. Both operations result in discharges of residual and waste materials to air and water.

Air Emissions--Volatile or gaseous pollutants are emitted to the atmosphere from stacks and by ventilation. In many cases, methods have been instituted to recover, neutralize, or otherwise control these emissions, but some residual emissions occur.

Water Effluents--Liquid and soluble chemicals are discharged to surface waters directly from process effluents or from holding ponds. Many effluent streams undergo biological or chemical/physical treatment before discharge to natural streams. Most waste streams enter flowing water; few, if any, munitions plants discharge directly to lakes or reservoirs.

Land Contaminants--A variety of existing and past Army activities have chemically polluted the soils of Army installations. Among these activities are:

- Manufacture, testing, and disposal of chemical munitions.
- Manufacture, testing, and disposal of conventional (explosive) munitions.
- Manufacture, testing, and disposal of insecticides, fungicides, and herbicides.

The testing and disposal of chemical munitions, conventional munitions, and pesticides has resulted in residual contamination of soils, either low-level contamination over wide areas or high-level pockets of contamination, such as that from burial of waste materials. Production of materials has been accompanied by wastewater discharges containing primary products, raw materials, intermediates, and by-products. Typically, wastewaters have been discharged to lined or unlined basins, in which pollutants are subject to biological or chemical degradation, evaporation, or adsorption on sediments. The degradation products of the original pollutants are often themselves residual pollutants.

A.2.1.2 Research Areas Considered

An enormous variety of research studies could conceivably contribute to the understanding and control of the environmental effects of Army chemicals. In practice, only certain areas have been identified as being within EPRD's mission, and even within these areas, certain categories of research have received much more attention than others. Categories of special interest to this study include chemistry, engineering, toxicology, and health effects (see Table A.2-1).

Chemistry and Engineering--The environmental chemistry of pollutants under actual environmental conditions is of considerable interest. Included in this research category are studies of oxidation,

Table A.2-1

EPRD PROGRAMS

- Toxicology and Health Effects
  - Epidemiology
  - Lifetime Tests in Mammals
  - 90-Day Tests in Mammals
  - Acute Tests in Mammals
  - Aquatic Field Surveys
  - Screening Aquatic Toxicity
  - Acute Aquatic Toxicity
  - Chronic Aquatic Toxicity
  - Mutagenesis
- Chemistry and Engineering
  - Environmental Chemistry
  - Source Strength Measurements
  - Sampling
  - Analytical Techniques
  - Hydrology
  - Hydrogeology
  - Treatment Efficacy
  - Chemical Identification

hydrolysis, photolysis, and microbial degradation of primary pollutants and characterization of degradation products. Also included are studies of evaporation and deposition, adsorption to sediments, leaching, and other intermedia transfers. Sometimes, physical transport research (for example, air dispersion) is also included.

Source strength measurements are designed to quantify the degree of discharge of pollutants to environmental media. At munitions plants, these take the form of measurements of the quality of discharged wastewaters and of the concentrations of volatile species in stacks and ventilation streams. Some information can be gathered from an input/output mass balance. For land pollutants, the concentrations in waste ponds can be measured or discharge records examined. Alternatively, groundwater concentrations in wells can be measured and fitted to a semi-empirical model (see Section A.6).

Pollutant characterization focuses on identifying and quantifying pollutants associated with various Army activities, and to some extent their degradation products as well. Both input/output analysis of the processes and sampling of discharges are employed in these studies.

Sampling is closely related to pollutant characterization, but is more concerned with searching for and quantifying concentrations of already-suspected contaminants. It is used particularly for characterizing the extent of land contamination, but could be used for air and water pollutants as well.

It is sometimes necessary to develop analytical techniques to ensure the success of the above programs, either because other chemicals interfere with existing techniques or because pollutant concentrations are too low for existing techniques.

The degree of hazard to human populations from water pollutants depends on the degree to which they are removed by water treatment plants. The efficacy of the treatment can be measured by laboratory simulations or field measurements (see Section A.5).

Hydrology entails the measurement of river flow volumes (discharges) and of the time it takes pollutants to reach populations at risk.

Hydrogeology examines groundwater flow rates and diffusion constants through the study of aquifer depth, thickness, and permeability, using test wells.

<u>Toxicology and Effects</u>--Epidemiology is not a traditional area for EPRD, but studies of munitions plant workers and other exposed populations could be done.

Mammalian toxicology is funded at three different levels: acute, subchronic (90-day) and lifetime. Lifetime tests include examination for carcinogenicity and reproductive effects. Aquatic toxicology is also funded at three levels: screening studies, full acute studies, and chronic (low-level) studies. Mutagenic assays are being used as possible indicators of carcinogenic potential. EPRD has begun toxicological studies in plants (phytotoxicity) and livestock.

Ecological studies, especially in the aquatic environment, involve field work at specific Army installations. The species in the vicinity are inventoried and their relationships studied. Concentrations of chemicals in media and tissues are measured, and the relationship between ecological parameters (such as species diversity) and pollutant loads is investigated. Studies of pollutants in model ecosystems could be included in this category, but such studies have not been emphasized.

Several areas of possible environmental research lie outside the domain of the present methodology. First, EPRD regularly conducts problem definition studies, which assess the existence and extent of specific problems. These lie outside the methodology because their value consists in sketching the broad boundaries of a problem rather than substantially reducing uncertainty about any particular phenomenon. Research on populations-at-risk to Army chemicals, regular monitoring of ambient levels, economic analysis of the severity of effects, methodology for pollution abatement, and treatment of pollutant-induced illness currently lie outside EPRD's principal areas of concern, although each, to some extent, is relevant to the intelligent setting of standards.

A.2.2 Implications of Research to Governmental Agencies

The objectives of research must be understood if the best course toward those objectives is to be selected. The stated purpose of this project is to aid in the setting of effective and rational standards for controlling pollution from Army activities. The standard-setting procedure is shared between the Army, which recommends criteria, the Enrivonmental Protection Agency, and various regional, state, and local regulatory bodies. The responsibility for meeting the standards is also the Army's (see Figure A.2-2).

A.2.2.1 Role of EPRD

The Environmental Protection Research Division (EPRD) is charged with the development of data bases to support criteria for emission and soil level standards for Army chemicals.

If toxicological thresholds exist for a particular chemical, below which no appreciable effects occur, then toxicological and ecological research determining those threshold levels is sufficient to set standards for ambient concentrations. However, to set performance

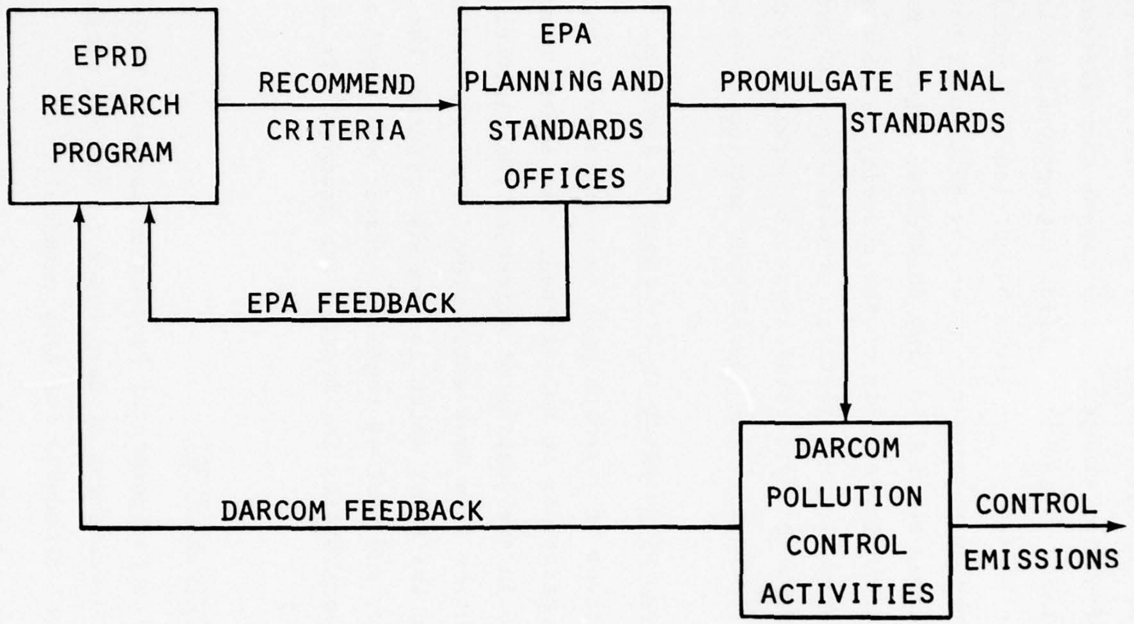

FIGURE A.2-2 STANDARD SETTING AND POLLUTION CONTROL standards for pollution abatement activities, it is necessary to understand much more about the releases and environmental behavior of the chemical. Furthermore, if some effects persist at low ambient levels, as is suspected for carcinogens, all the relationships in setting an acceptable level of risk are relevant research subjects.

EPRD's first responsibility is to recommend standards that provide a margin of safety for environmental protection. But safety is a relative term, and for effects with no known threshold, some hazard must be tolerated unless zero-discharge standards are stringently enforced. The EPRD must also consider the difficulties of unrealistically stringent standards, as there are economic and technical problems of abatement that offset the benefits of the strict standards.

A.2.2.2 Role of EPA

The Environmental Protection Agency promulgates and enforces environmental standards for Army chemicals. It may accept or ignore EPRD recommendations dependent largely on the thoroughness and credibility of the EPRD data base.

Although environmental statutes and regulatory precedent place certain constraints on the standard-setting procedure, we can reasonably assume some features of EPA's strategy in dealing with criteria recommended by EPRD.

The EPA is charged with maintaining environmental health and welfare. Consequently, EPA cannot permit any level of chemical discharge to the environment without adequate assurance that hazards are low. However, EPA may accept some low, but nonzero, "acceptable hazard" as an unavoidable penalty for obtaining the benefits of chemical usage. In such a case, EPA requires performance standards from the Army that are relatively certain to reduce the ambient concentrations and associated hazards to this acceptable level. When the standards recommended by EPRD are based on complete documentation of a chemical's hazards and the means to reduce them, EPA can readily adopt such standards. However, when EPRD's research base is incomplete, uncertainties exist as to the current hazard and the hazard remaining after abatement, and EPA's only alternative is to require a more stringent standard, one that will protect the environment from the estimated upper limit of the hazard.

For example, suppose that an assumed safe level of discharge (the criterion) is as shown in the "test tubes" of Figure A.2-3, but the range of uncertainty is large. EPA would tend to set the "safe" safe level as a standard (left tube). Research tends to narrow the range of uncertainty and to increase the "safe" safe level to an "acceptable" safe level (right tube).

Clearly, then the reduction of the uncertainty in the hazard is a primary goal of EPRD, to avoid on the one hand overly expensive abatement strategies, and, on the other, unexpectedly high hazards should EPA accept the initially recommended criteria.

A.2.2.3 Pollution Abatement

Research on or responsibility for pollution abatement is not part of EPRD's mission. However, it is in the best interests of the Army, and ultimately of the nation, for EPRD to recommend the least burdensome standards consonant with environmental protection. The costs of developing and implementing methods of pollution abatement should be balanced against both the health and welfare benefits resulting from environmental control and the costs of environmental research. For example, in rare cases it may be possible to achieve a stricter standard than actually necessary because it is cheaper to control the pollutant than to conduct research to support a less stringent standard. On the other hand, it may be possible to demonstrate that the likelihood of a pollutant producing significant effects is so low, even in the face of residual uncertainty, that extensive cleanup programs are not justified on a cost/risk/benefit basis.

A.2.2.4 Role of DARCOM

The Army Materiel Development and Readiness Command (DARCOM--formerly the Army Materiel Command) is charged with research and development of pollution control technology for munitions plants and

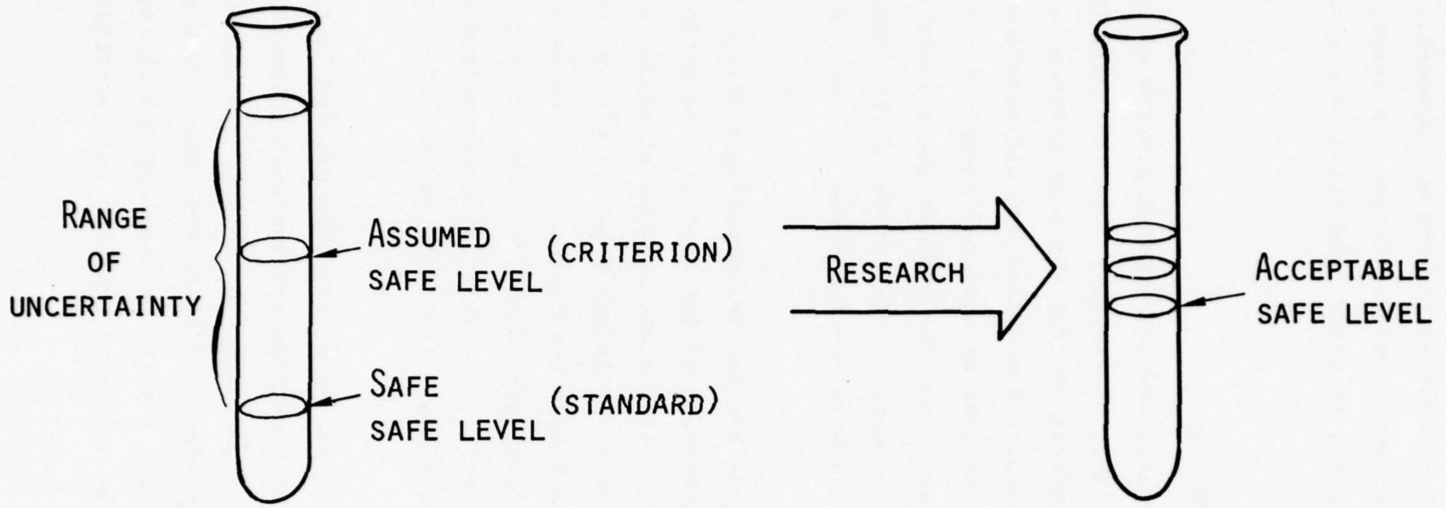

FIGURE A.2-3 UNCERTAINTY IN CRITERIA AND STANDARDS for installation restoration. DARCOM must meet all environmental standards imposed on it, given the necessary resources. However, it is reasonable to presume that DARCOM would prefer to meet the least stringent standards consistent with safety, to avoid committing resources that could be better used elsewhere.

A.2.2.5 Value of Research

The Army research and development program addressed by this report is designed to reduce uncertainty about the effectiveness of alternative pollutant standards so that the best balance between the conflicting goals of environmental protection and minimization of abatement costs (consistent with the goal of national security) can be struck (Figure A.2-4). The more exactly one can predict the effects of a given level of pollution and the more certain one can be of the levels resulting from a given discharge, the more precisely one can set a standard with confidence.

EPRD is responsible for recommending criteria for standards that are in the best interests of the Army and the nation. Research is necessary to assure that the recommended standards are based on the best possible knowledge of pollutant behavior within resource limits. Because there are many more uncertainties to reduce than there is money to reduce them, the Army should select those research programs that most reduce uncertainty per unit cost of research within constraints of total available budget and minimum standards for the significance of the results.

The basic research prioritization problem is thus one of balancing the costs of research programs and abatement procedures against the risks of setting standards that are too lenient, and the benefits of the production and use of munitions and other Army chemical products. This qualitative discussion of the basic methodology underlying the prioritization process will be made more explicit and quantitative in the following sections.

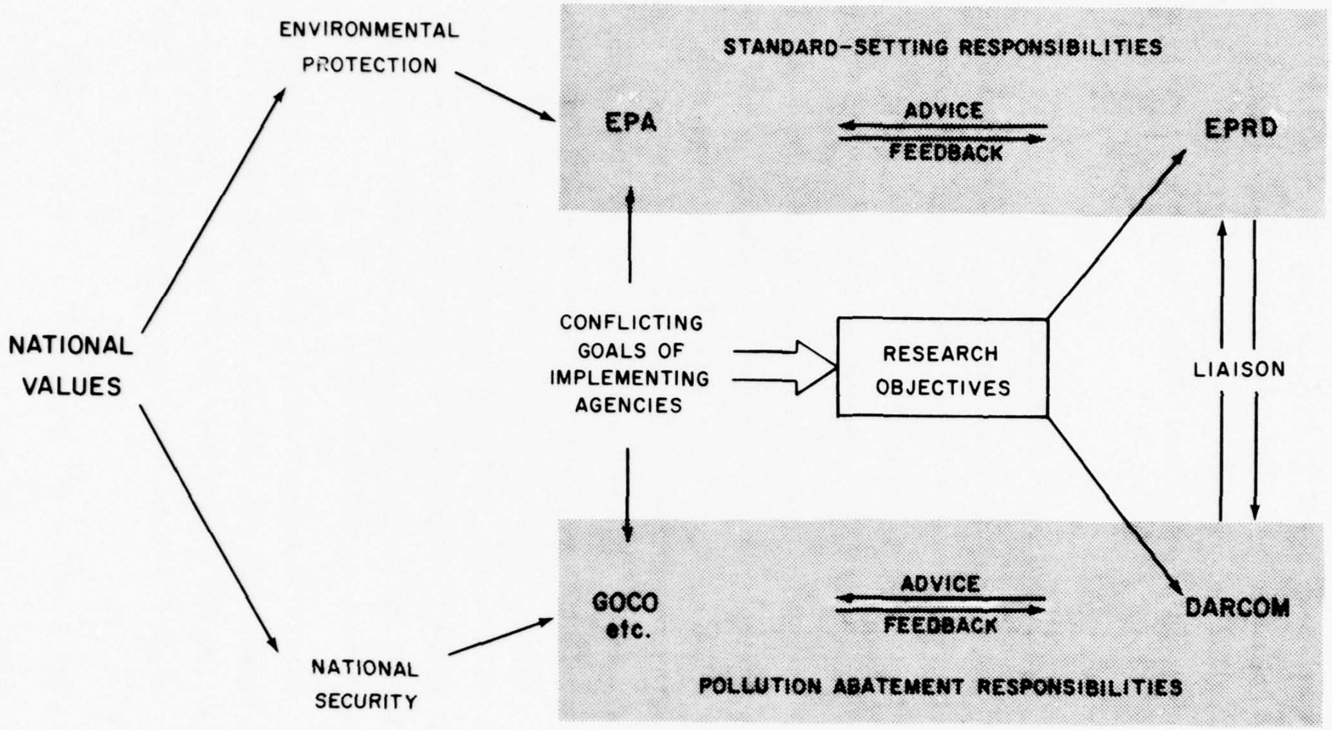

FIGURE A.2-4 RATIONALE FOR RESEARCH

A.2.3 Criteria for Selecting a Research Program

The criteria for selecting one research program over a competitor are the estimated hazard posed by a pollutant, the uncertainty in the hazard that can be reduced by a given research study, the cost and effectiveness of pollution abatement, and the value (benefit) of the Army activities producing the pollutant. These concepts are more carefully defined below.

A.2.3.1 The Concepts of Hazard and Risk

The terms hazard and risk have been used almost interchangeably to describe the severity of the unwanted effects of pollution. More precise definitions were used for this project. These definitions do not necessarily conform with other researchers' use of the terms.

Risk is defined as the probability that any individual member of a population will incur a specific adverse effect from a specific pollutant. Thus, it could be said that Mr. Jones runs a 1% risk of developing skin cancer from Lewisite oxide over the next year. Risks can vary markedly from individual to individual and from group to group, depending on such factors as degree of exposure and susceptibility. Some standards, such as ambient quality standards, are generated by the desire to limit risk to any individual to some specified or implicit low level. In some cases, this extends to a zero-risk concept, which implies either zero exposure or the existence of a threshold, that is, a level of exposure below which no effects occur.

Hazard is defined as the integral of all risks over an entire exposed population, for example, all the people in the United States. Suppose 100,000 people were at 1% risk to emphysema, 10 million were at 0.05% risk, and 200 million were at 0.0001% risk. Then the hazard would be

$$10^5 \times 10^{-2} + 10^7 \times 5 \times 10^{-4} + 2 \times 10^8 \times 10^{-6}$$

$$= 10^3 + 5 \times 10^3 + 2 \times 10^2$$

$$= 6,200$$

which means that over 6,000 cases of emphysema could be expected in the total population. Many standards are set on the basis of an "acceptable hazard," although the acceptable level may not be explicitly defined. For example, automobile safety standards and other regulations (speed limits, and so on) have limited annual traffic fatalities to about 50,000. This level is apparently considered acceptable, given the cost and inconvenience of imposing stricter standards. Of course, it is well known that different answers are given for what hazards are acceptable depending on whether the risks are voluntary or involuntary, and whether the risks and benefits accrue to the same or different populations.

Risk and hazard are not confined to human effects. A fish can be at risk of acute fatal toxic effects from a given pollutant, and the entire exposed fish population experiences a corresponding hazard over a year's time. However, a 1% risk of death in fish is not equivalent to a 1% risk of death in humans, just as an expected hazard of 2,000 cases of human dermatitis is not equivalent to 2,000 expected cases of chronic arteriosclerosis. To estimate the total hazard of all the effects attributable to a chemical requires that a value be placed on each effect to make the resulting hazard-values expressible in common terms. This difficult problem of effect valuation will be discussed further in Section A.3.

A.2.3.2 Reduction of Hazard Uncertainty

To this point, the ability to estimate the hazards posed by a particular pollutant has been assumed. However, it is evident that even in the best of circumstances, the quantitative hazard cannot be estimated very accurately. After years of research on cigarette smoking, experts have estimated the hazard of smoking to be in the vicinity of 50,000 lung cancer deaths per year, but this "best estimate" is uncertain by 10,000 or 20,000 per year because the exact cause of a particular lung cancer may be ambiguous. Uncertainty in the hazard is the principal reason for doing research; otherwise a cost-risk-benefit equation between hazard and cost of abatement can be used to set standards, and no further research is necessary.

One way of expressing uncertainty is in terms of "confidence limits." In the example above, it is reasonably certain that smoking cancers fall in the range 30,000 to 70,000 per year; that is, the lower confidence level is 30,000 and the upper confidence level 70,000. But it must be emphasized that these confidence limits are subjective in the Bayesian sense (see Section A.7), and are not entirely equivalent to objective confidence limits that would be computed from a series of experiments. Thus, to continue with the example above, if the smoking cancer uncertainty were to be described in terms of "95% confidence limits," this implies that experts are betting 20 to 1 that the true answer is within the range of 30,000 to 70,000 per year, rather than that the "real" probability is 95%.

However, in priority-setting problems, where uncertainties are typically very large, it is often more convenient to think in terms of an "uncertainty factor" rather than of the more usual ±40%. An uncertainty factor is defined as the quantity by which the best estimate is divided or multiplied to express the lower and upper confidence levels, respectively. For example, if the best estimate of the hazard is expressed as 1,000 deaths per year, an uncertainty factor of 10 gives lower and upper confidence limits of 100 and 10,000. Although it is not necessary to assume an underlying probability distribution--and even may be dangerous to do so--the uncertainty factor concept is consistent with an underlying log-normal distribution.

Uncertainty in hazard is the key criterion for standards research. Uncertainty in hazard exists between the upper confidence limit and the best estimate of the hazard. For safety, the Army must assume that the upper confidence limit rather than the best estimate is the true hazard. If an acceptable hazard has been determined, explicitly or implicitly, then the standard can be set to reduce the upper bound of hazard to the acceptable hazard. Symbolically, if HU is the hazard uncertainty, H^* is the acceptable hazard, and S is the operation of reducing the hazard through setting the standard, then

$$S(HU) \rightarrow H^*$$

This will usually result in a more stringent standard than necessary, because the true original hazard is much more likely to be near the best estimate than near the upper confidence limit (see Figure A.2-5). Therefore, the reduction of the hazard uncertainty by a given factor will usually mean that abatement requirements can be relaxed. Said in another way, good research can reduce the safety factor in setting a standard.

Notice, however, that a given research program, for example, a toxicology study, does not work directly on uncertainty in hazard but instead on a component uncertainty, namely, the uncertainty surrounding the levels of exposure at which specific effects occur. A reduction of an uncertainty factor in toxicology from 10 to 5 (a twofold change) could result in a hazard uncertainty factor change from 40 to 30 (only a 1/3 change). Therefore, one must determine which research programs are likely to change the overall hazard uncertainty most.

A.2.3.3 Cost and Effectiveness of Research

The effectiveness of a program, that is, the degree to which it reduces hazard uncertainty, is not the only criterion for choosing between competing research studies--cost must be considered. If two research programs reduce hazard uncertainty equally--say a carcinogenic test on TNT and an environmental chemistry (half-life) test on cyclohexanone, and one program (the carcinogenic test) is several times as expensive as the other, then the chemistry program would clearly be preferred. However, the supposition above is that the hazard-uncertainty reduction is the same in both programs. Since the two programs enter the hazard estimate in different ways, a tenfold uncertainty reduction in half-life might be required to have the same effect on hazard uncertainty as only a twofold reduction in carcinogenic uncertainty. Therefore, the expected effectiveness of a research program in terms of uncertainty reduction is as much a criterion for selection as is its cost.

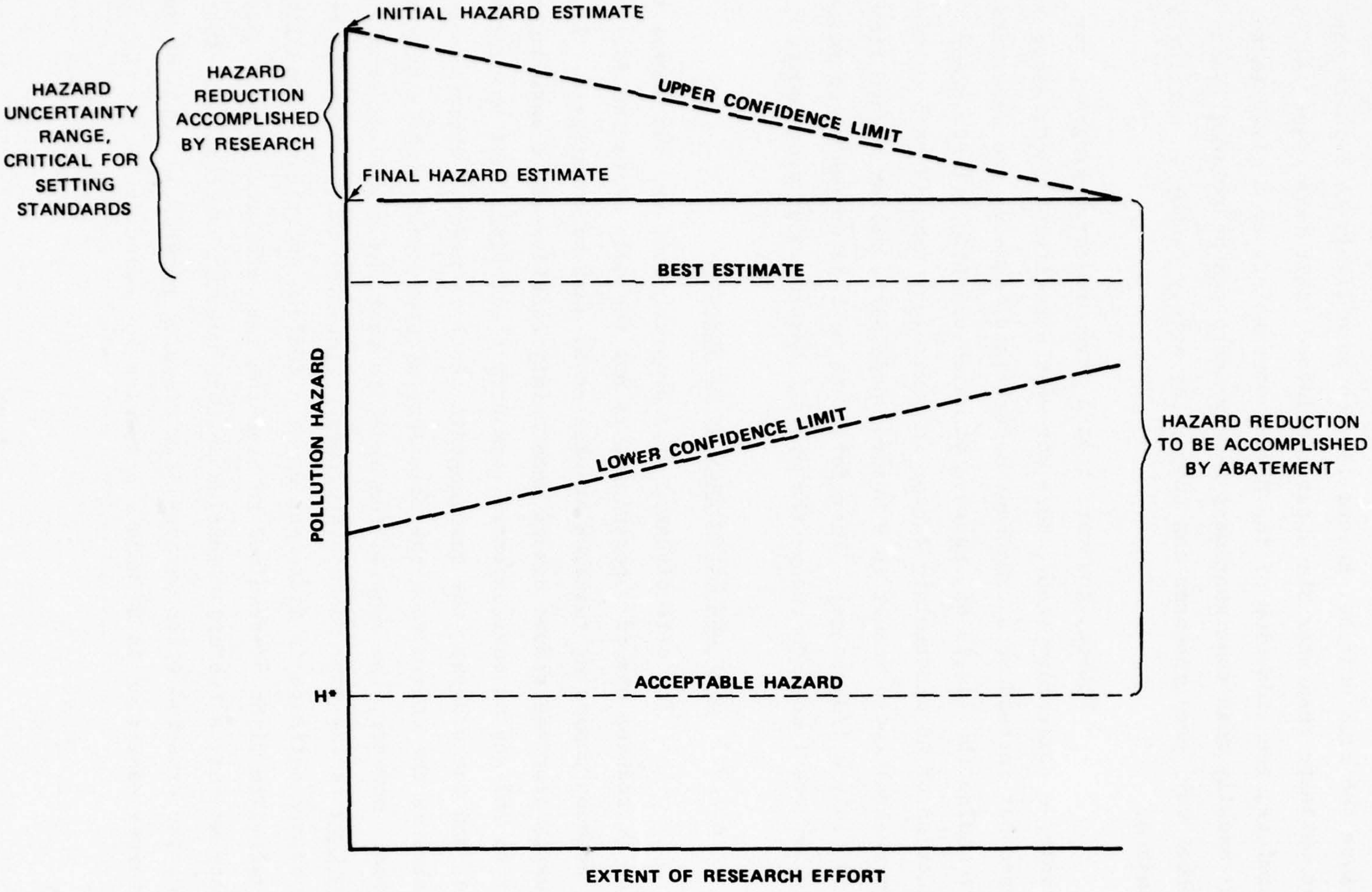

FIGURE A.2-5 EFFECT OF REDUCTION IN HAZARD UNCERTAINTY ON STANDARDS

A.2.3.4 Other Criteria

The above criteria are the principal quantitative inputs to the research priority allocation methodology. Not included in the methodology are other quantifiable and nonquantifiable criteria that may have impacts on the ultimate selection of a research program.

The cost of abatement activities, although the responsibility of DARCOM, not EPRD, is important. Low abatement costs for high pollutant control could preclude a requirement for further research. High abatement costs have the opposite effect.

The effectiveness of abatement activities, in terms of reduction in discharge, for a given investment, is also a criterion, because less effective abatement methods are in greater need of a justification for a less strict standard. Figure A.2-6 shows a theoretical trade-off curve between hazard costs (lax standards) and cleanup costs (stringent standards) that shows how uncertainty in hazard results in suboptimal standard-setting. However, few data on abatement costs are available for specific Army pollutants. Control procedures which abate one pollutant often abate others as well. Thus, these criteria should be used as a secondary qualitative set rather than in the quantitative methodology.

The value of the Army activities producing the pollution is another criterion. For example, if a plant is producing a primer that has a polluting by-product, and that primer is not greatly needed, or can be replaced with a less polluting substitute, the simplest solution is to stop production of the primer rather than implement pollution controls or do research toward clarifying standards. Again, data on the value of Army activities are relatively unavailable, and decisions can only be influenced qualitatively.

A host of nonquantifiable (or quantifiable only with difficulty) criteria can be applied to the final allocation. Some programs are directed. Politics and public relations are motivators. Others are related and are best done in concert. Requirements beyond the control of EPRD that standards be promulgated at a specific time may influence the selection of candidate studies.

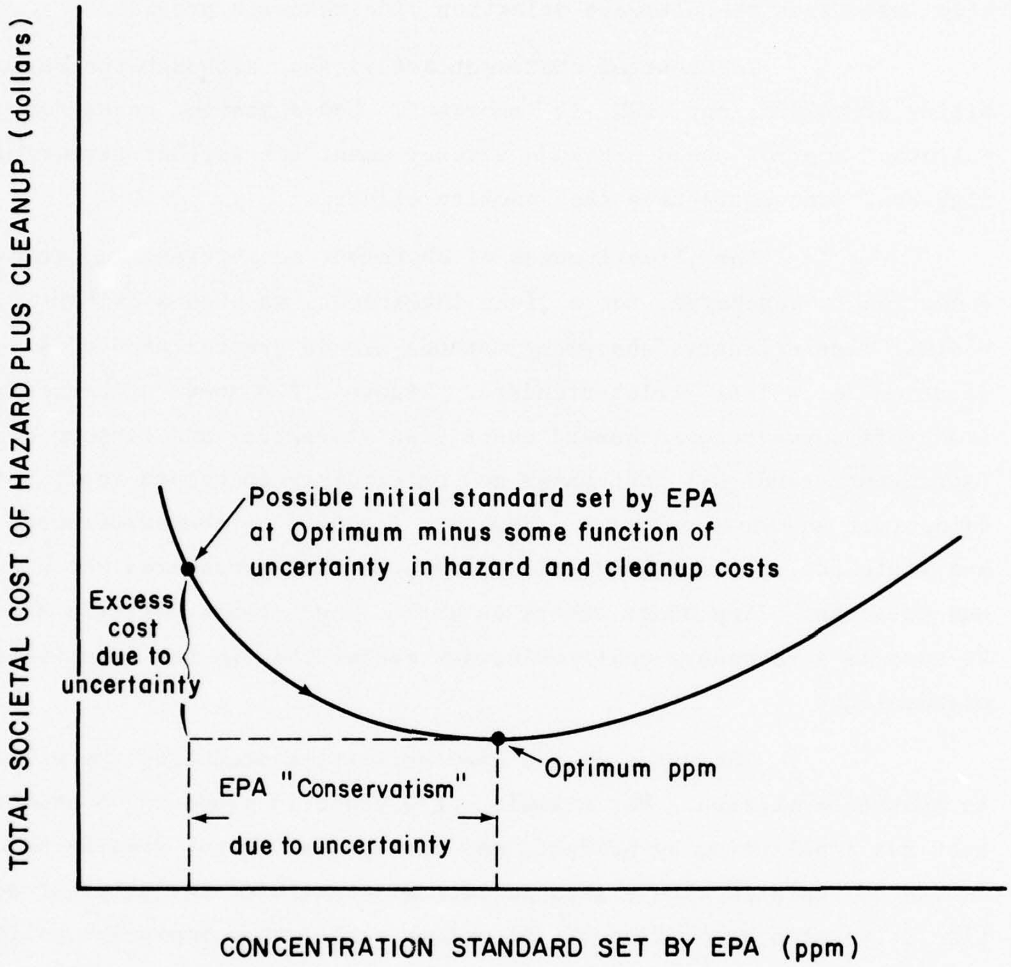

FIGURE A.2-6 ILLUSTRATION OF HOW R&D CAN REDUCE UNCERTAINTY IN HAZARD OR CLEANUP COSTS AND THUS HELP TO ACHIEVE A MORE ECONOMIC CONCENTRATION STANDARD

A.2.3.5 Information Constraints

A fully satisfying and logical allocation of research resources would be possible if all criteria could be applied with confidence to well-defined research programs. In practice, it is not economically feasible to gather all the information needed to make such a confident allocation.

Information to estimate hazard is spotty and uncertain. Both the kinds of phenomena to be treated and the quantitative data for describing them are often very uncertain. When virtually nothing is known about a possibly important phenomenon, it is nearly impossible to put a meaningful description of it into the hazard estimation system. Such gaps are clues that research is necessary, but they give little guidance on what resources should be devoted.

A second area of difficulty is the detail in which research programs can be described. For example, ideally, the proposed allocation system works at the level in which a specific test (such as chronic toxicity in mammals) is applied to a specific chemical, and is described in detail in terms of its cost and the expected accuracy of its results (for example, it will fix the slope of the dose-response curve for CNS disturbance within a factor of 3). However, funds are not always allocated at this level of detail. A program of toxicity testing on several chemicals, including range-finding tests, is often packaged together. Moreover, it is usually difficult to predict the outcome of a research program in reducing uncertainty.

A.2.4 Quantitative Models for Allocation

The principal quantitative criteria for research program selection are the reduction in hazard uncertainty expected upon completion of the program and the program cost. Translation of this concept into a systematic methodology requires first a careful definition of hazard and uncertainty and then specifications on how they are combined with program costs to generate an index of priority for program selection.

A.2.4.1 Definition of Hazards

The hazard created by a chemical can be defined in terms of the expected number of adverse effects in the total exposed population. For Army chemicals, the hazards of concern are the biological effects in all exposed species from munitions plant discharges and land contamination. In practice, the population exposed to these discharges are usually all located relatively near the munitions plants or contaminated installations.

For humans, biological effects include acute toxicity, especially fatalities, and long-term toxicity, such as carcinogenicity or cardiovascular effects. In the case of economically important species--decreases in yield. Reproductive failure, species avoidance of its normal habitat, ecosystem disturbance are biological effects of potential importance, but information on these effects is usually so scanty as to be virtually unusable.

The most controversial feature of the current definition of hazard is the dollar valuation of effects. For convenience, hazard is expressed in terms of dollars, based on various treatments of the value of human life, disease, and economic worth of lower life forms. However, it is the relative values that are important, and these can be varied to account for different relative value systems.

Thus, a simplistic but useful view of hazard is the total economic burden placed on the environment by the chemical under consideration.

The details of calculating an estimated hazard will be given in Sections A.3-A.6, but it is important at this point to understand that hazards can be expressed at many levels of aggregation.

The most disaggregated and basic unit of hazard is the hazard due to a specific chemical, i, discharged from a specific location, j (munitions plant or other installation), into a specific environmental medium, m, and causing a specific effect, ℓ, in a specific group, k, of a given species (population type), at risk, n. For example, using alphanumeric codes for the subscripts, one can estimate the hazard due to the discharge of nitroglycerin (i = NG) from the Radford Army Ammunition Plant (j = RAD) into river water (m = H2O) and causing fish kills (ℓ = FKL) in the fish (n = FSH) in the first reservoir downstream of the discharge point (k = 1). This hazard, known as a "six-subscript hazard," will be designated by the symbol $H_{ijmnk\ell}$.*

If one wishes to know the hazard to all the population groups (k) within a population type (n) with all other subscripts specified (that is, for a given chemical, location, medium, and effect), then he should sum or aggregate over the index k. The resulting hazard is one of six different kinds of aggregate "five-subscript hazards;" it is designated by a set of subscripts that omits the summed subscript:

$$H_{ijmn\ell} = \sum_{k} H_{ijmnk\ell} \quad .$$

For example, $H_{ijmn\ell}$ could represent the hazard to all fish downstream of Radford from the acute toxicity of nitroglycerin. Other aggregations are equally possible (all effects in the human population in Brighton, Colorado, from discharges of DIMP into groundwater at Rocky Mountain Arsenal, or cancers to humans in Chattanooga from the river water discharges of all the chemicals at the Volunteer AAP).

Aggregation can occur at higher levels by summing over additional subscripts to obtain four-, three-, two-, and one-subscript hazards. For example, the total of all hazards for a given chemical, H_i, and the total hazard from all chemicals at a given location, H_j, are particularly useful aggregations. The zero-subscript hazard, H, is the total of all (estimated) hazards from all (included) Army activities.

Six-subscript hazards are the cells of a six-dimensional matrix; five-subscript hazards are the row totals, making up six different five-dimensional matrices, and so on. However, it is extremely important to note that many of the cells are empty, that is $H_{ijmnk\ell} = 0$.

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*The order of subscripts is not alphabetic because of an early decision on the logic and mnemonics of subscript definition.

In fact, most of the cells are empty, because not every chemical is discharged into any one medium, and so on. It will become evident later that this sparse nature of the matrix creates both problems and opportunities in data processing.

A.2.4.2 Definition of Uncertainties

As will be shown later, each of the six-subscript hazards can be estimated on the basis of a function of several component variables, such as quantity of chemical discharged, environmental half-life, or slope of a dose-response relationship. With each of the component variables, there is a range of uncertainty in value about the best estimate, as indicated by the three levels in the "test-tubes" of Figure A.2-7, which indicate the best estimate and the upper and lower bounds. More precise definitions of these uncertainties and ways of estimating them are discussed in Section A.7. For the moment, however, it suffices to state that the uncertainties in the component variables cause a corresponding uncertainty in the estimated hazard, as represented by the levels in the beaker of Figure A.2-7. The way the uncertainties combine is known as the propagation of uncertainty, and details of this process will also be given later. The right-hand part of Figure A.2-7 indicates only that the answer to the question of uncertainty propagation is not simple and obvious.

The important fact to recognize at this point is that the uncertainty in a six-subscript hazard can be estimated from those of its component variables, and that the hazard uncertainties can in turn be propagated to aggregated hazards. Furthermore, this can be done both for the current state of information and for a postulated future state of information, after an experiment on one of the component variables has been completed and its uncertainty reduced.

Several ways in which hazard uncertainty can be expressed are discussed in more detail in Section A.7. The most convenient way of expressing hazard uncertainty propagated from component uncertainties is as the standard deviation of a set of hazard estimates generated by a probabilistic simulation (the so-called Monte Carlo technique). Let the standard deviation in a six-subscript hazard $H_{ijmnk\ell}$ be represented

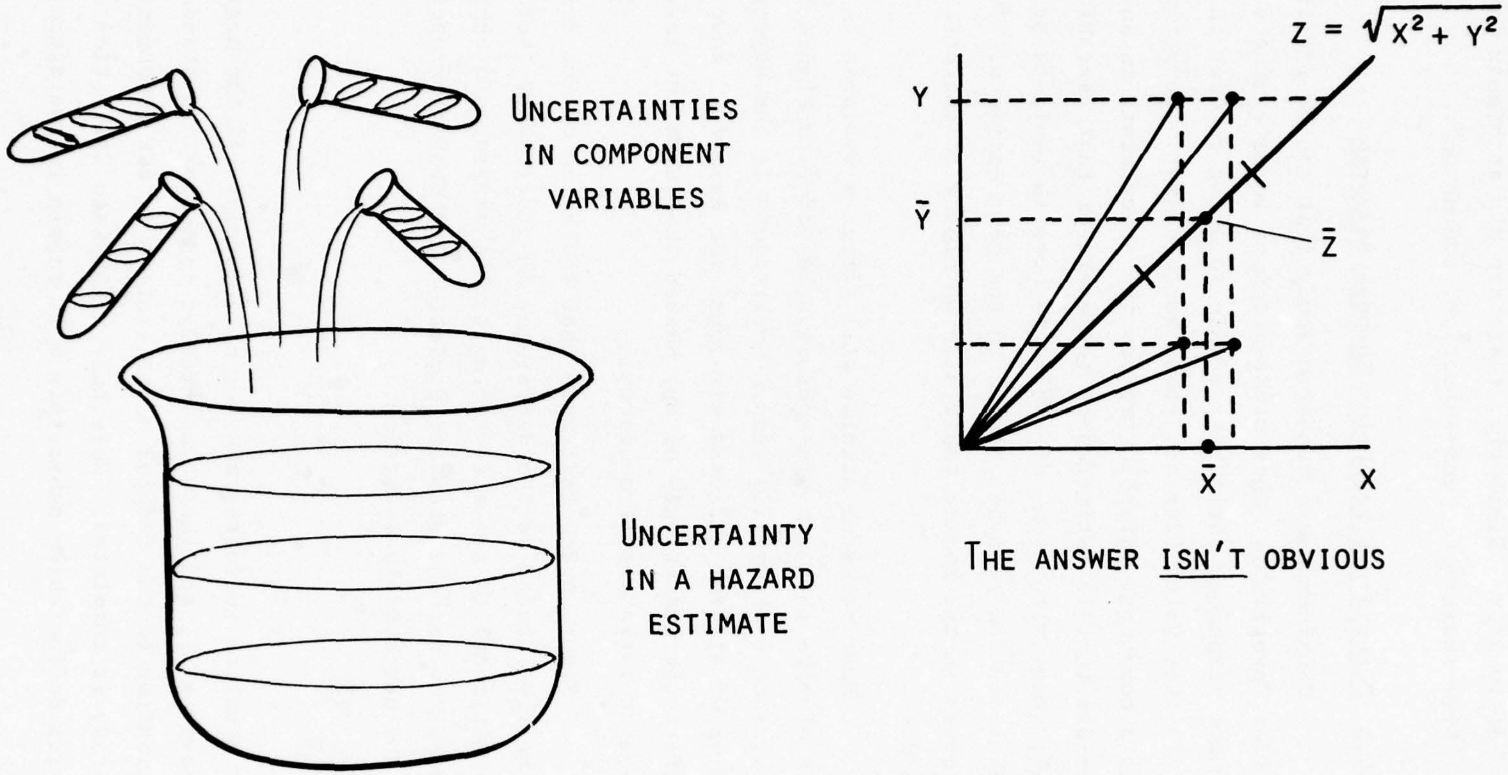

FIGURE A.2-7 PROPAGATING UNCERTAINTY — THE IDEA by $\sigma_{ijmnk\ell}$. This standard deviation will have the same units as does the hazard, namely $/yr. Similarly, there are σ's at higher levels of aggregation (five-subscript, four-subscript, and so on).

A.2.4.3 Uncertainty Reduction Through Research

Consider now a research study that can be identified by an index p (for "program"). This study attempts to determine a value for one or more component variables, and in so doing reduces the uncertainty in that value (for any study worth doing). Reduction of uncertainty in a component variable reduces the uncertainty in any six-subscript hazard that is estimated on the basis of that variable. (In Figure A.2-7, imagine that one of the test-tubes is replaced by another with the upper and lower levels closer to the best estimate. The upper and lower levels in the beaker would also be closer to the best estimate of the hazard.)

Most research studies will affect a variable that enters the estimate of more than one six-subscript hazard (see Figure A.2-8). Consequently, such a study will reduce uncertainty in the aggregate hazard made up of all the affected six-subscript hazards. However, it will not affect the uncertainty of any hazard that does not involve one of the component variables it measures.

Figure A.2-8 indicates that the value of the research study is directly related to the difference in uncertainty (before and after the experiment) in the affected aggregate hazard. To express this quantitatively, we use the standard deviation expression of uncertainty and define the uncertainty reduction as

$$\Delta\sigma_p = \sigma_{\sim} - \sigma_{\sim}^{p}$$

where the $\sim$ notation indicates the set of subscripts in the aggregate hazard (zero to six), and the p superscript indicates the standard deviation corresponding to the reduced uncertainties in the component variables after the study is completed. Note that a complete definition of the study, p, will define which subscripts will remain in the aggregate hazard.

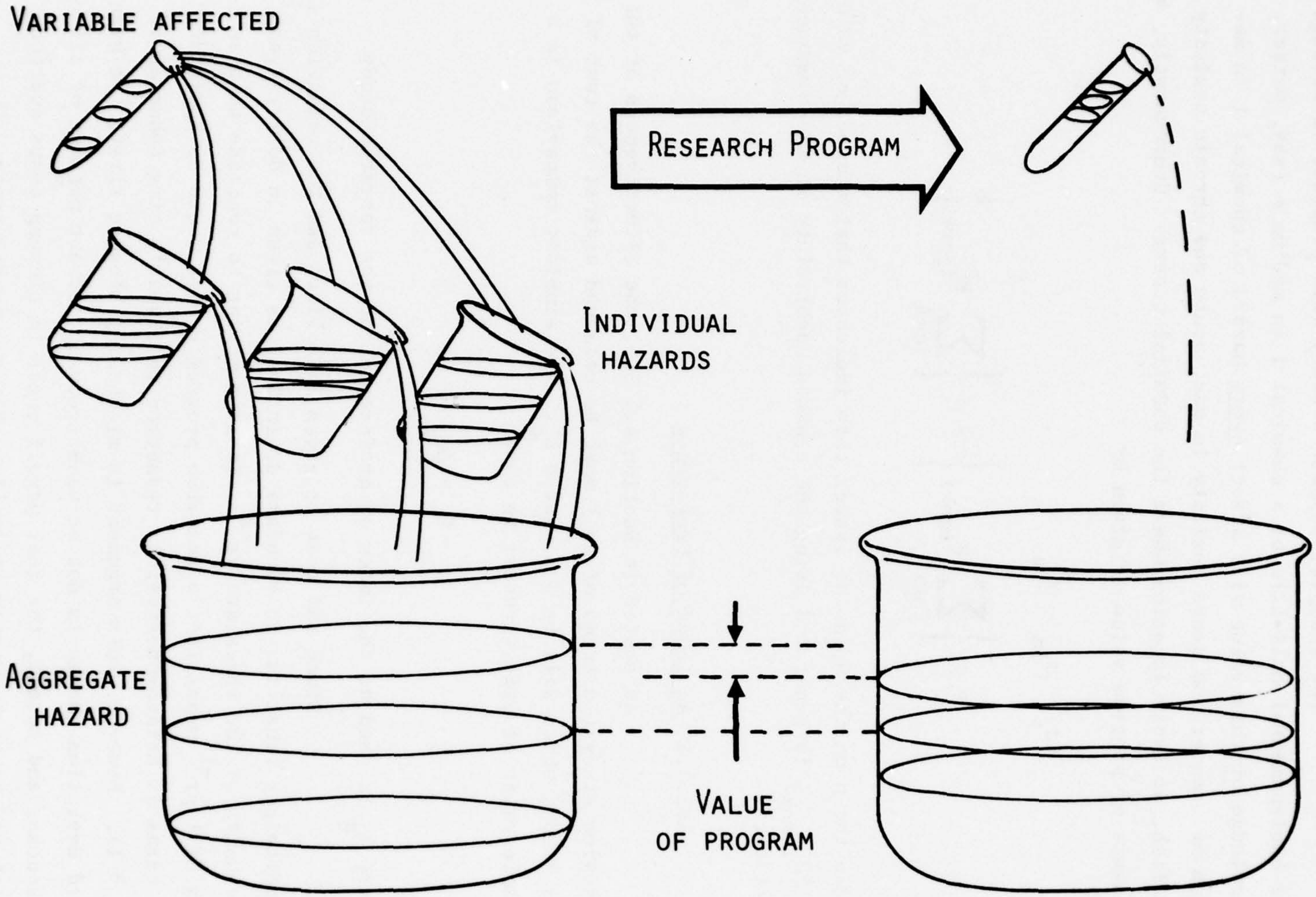

FIGURE A.2-8 EVALUATING A RESEARCH PROGRAM — THE IDEA

For example, suppose a study were proposed to measure the environmental half-life of a chemical i in medium m (say, water). Knowledge of this value will affect <u>every</u> hazard of chemical i in medium m: cancer and acute toxicity in man, acute and chronic toxicity in fish, at every location where the chemical occurs. Consequently, a measure of program value is given by

$$\begin{aligned}\Delta\sigma_p &= \sigma_{im} - \sigma^p_{im} \\ &= \sigma\left\{\sum_{jnk\ell} H_{imnk\ell}\right\} - \sigma\left\{\sum_{jnk\ell} H^p_{ijmnk\ell}\right\}\end{aligned}$$

where the p on the H in the latter term indicates that the set of values of $\Sigma H_{ijmnk\ell}$ is generated using the reduced uncertainty in the component variables.

A.2.4.4 An Index of Preference

As stated in Section A.2.3.3, the effectiveness of the research study (in terms of $\Delta\sigma_p$) must be balanced against the cost of the study, which will be designated C_p. The simplest comparison is a simple ratio of effectiveness to cost:

$$I_p = \Delta\sigma_p / C_p$$

where I_p is used as the index of preference for the research study.

Since the cost is given in dollars and the reduction in uncertainty (that is, in standard deviation) is given in dollars/year, the units of the index are yr^{-1}. It is tempting to conclude that an index of 1 yr^{-1} means that a research program's cost would be "paid off" in terms of hazard-uncertainty reduction in a year's time (shorter if $I_p > 1$). However, this argument is misleading because first, the standard deviation change is not an unambiguously correct measure of effectiveness, and second, the real payoff comes in cleanup costs averted, which may be much greater or smaller than the hazard costs.

Once the index I_p has been generated for a series of candidate research studies, a ranked list of studies can be prepared with the highest I_p's at the top. This list can then be examined to see if the high-ranking studies meet all of EPRD's subjective criteria for selection. Once the list has been refined by removing or reordering some studies on the basis of these subjective criteria, the final selection can be made from the highest ranking studies up to the point that exhausts the discretionary budget (B) to be allocated in the current funding cycle. Quantitatively, a constraint is put on the allocation:

$$\sum_p C_p \leq B \quad .$$

Notice that it is possible that selecting a costly study at some place on the list might cause the sum of costs to exceed the budget, whereas selecting a lower-ranking one might not. In such a situation different selection of studies might better fit the budget, leaving some higher-ranking studies for the next budget cycle.

A.2.4.5 The Allocation Methodology: A Tool of Decision Making

The methodology outlined above represents a logical approach to the allocation of research funds to the extent that it is able to quantify and systematize the decision criteria for selecting one study over another. It is thus potentially a valuable tool in decision making. However, it is limited in usefulness when used without caution or judgment. There are too many subjective criteria that are not treated, and too many assumptions, approximations, and expedient solutions in the methodology for it to be used without severe and continuous questioning. It is anticipated that many studies recommended by the methodology will be found unsuitable for selection. The methodology should be most valuable in the identification of studies and target chemicals not immediately obvious to busy managers. A valuable by-product will be the data base required for operation.

A.3 THE HAZARD ESTIMATING AND RANKING SYSTEM

In the course of developing the allocation methodology, it is necessary to develop a systematic way of estimating the hazard associated with each chemical pollutant from Army activities. These hazard estimates are a measure, however imprecise, of the total deleterious effects of the munitions plant discharges and land contamination resulting from these activities. They are also interesting in themselves from two viewpoints:

- Relative importance of Army chemical hazards with respect to one another.
- Importance of Army chemical hazards with respect to other hazards, such as those of civilian chemicals.

In recognition of these useful products of hazard estimation, an intermediate objective of this study was to produce a hazard ranking of Army chemicals and to additionally rate several civilian chemicals as points of comparison with the Army rankings.

Section A.3 describes the broad fundamentals of the system developed to estimate and rank the hazards of chemical pollutants. Detailed descriptions of each of the major modules of the system are presented in the succeeding three sections (A.4, A.5, and A.6).

A.3.1 Fundamentals of Hazard Estimating and Ranking System

A.3.1.1 Classification of Pollution Problems

The Army has divided its chemical pollution problems into three major areas: air pollutants from munitions plants, water pollutants from munitions plants, and land contaminants on installations. The division of chemicals by these categories is shown in Table A.3.1. Although it was originally anticipated that there would be a great deal of mingling of these problems, especially due to intermedia transfer of pollutants, it has been found that the hazard estimating and ranking system can be separated into three major modules, with only occasional need to intersect the

Table A.3-1

CHEMICAL POLLUTANTS

Code*	Water	Code	Land
NG	Nitroglycerin	TDG	Thiodiglycol
TNT	2,4,6-Trinitrotoluene	LWO	Lewisite oxide
NGU	Nitroguanidine	MPA	Methyl phosphonic acid
TNR	Trinitroresorcinol	IMP	Isopropyl methylphosphonate
TZ	Tetracene	DMP	Diisopropyl methylphosphonate
PBS	Lead styphnate	CHL	Chlorates
PET	PETN	DPD	Dicyclopentadiene
WPH	White phosphorus		
RDX	RDX		
HMX	HMX		
NDP	o-Nitrodiphenylamine		Civilian
13D	Glycerol-1,3-dinitrate		
1MG	Glycerol-1-nitrate	BNZ	Benzene
2MG	Glycerol-2-nitrate	NBZ	Nitrobenzene
26D	2,6-Dinitrotoluene	PVC	Polyvinyl chloride
24D	2,4-Dinitrotoluene	CTC	Carbon tetrachloride
4AD	4-Amino-2,6-dinitrotoluene	DDM	Dichlorodifluoromethane
2AD	2-Amino-4,6-dinitrotoluene		
12D	Glycerol-1,2-dinitrate		
CHX	Cyclohexanone		
HEX	Hexamine		
SEX	SEX		
	Air		
MN	Methyl nitrate		
TNM	Tetranitromethane		
NM	Nitromethane		
MNT	Mononitrotoluenes		

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[*] Mnemonic for data processing.

three. With respect to munitions plants, pollutants that are originally discharged to the air seem to exert the majort of their effects through the air medium. The same is usually true for water pollutants, although a few seem to have a significant evaporation rate to the air. For land contaminants, the principal route of concern seems to be groundwater, at least at RMA. However, inclusion of a transfer to surface water and computation of the effects in that medium is indicated there.

A.3.1.2 Major Components of the System Model

An overview of the hazard estimating and ranking system is shown in Figure A.3-1, which indicates that several components of the system are common to all three modules. These major components are discussed in the following paragraphs.

Sources--Average emissions rates to air and effluents to water from munitions plants are estimated in kg/yr. The rate of leaching of land contaminants into groundwater is estimated in kg/yr for a recent year (usually 1974). An equivalent soil pollutant inventory, in kg, can be estimated on the basis of the estimated linear transfer coefficients out of the inventory in $(yr)^{-1}$. The rate of introduction into surface water by percolation from groundwater is estimated from the aquifer flow volumes and the pollutant concentrations along the river bank, also in kg/yr. The outputs of the source component are the discharge rates to the media. The major sources considered are tabulated in Table A.3-2.

Transport--The transport, transformation, and transfer models simulate processes that are going on simultaneously, but it is convenient to think of them acting separately. The transport models simulate the distribution of chemicals from assumed point* sources to the geographical locations of populations-at-risk, and estimate the resulting concentrations at those locations. In air, a Gaussian diffusion type of model is used with detailed meteorological frequency data on wind speed

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*Line, in the case of groundwater to surface water transfer.

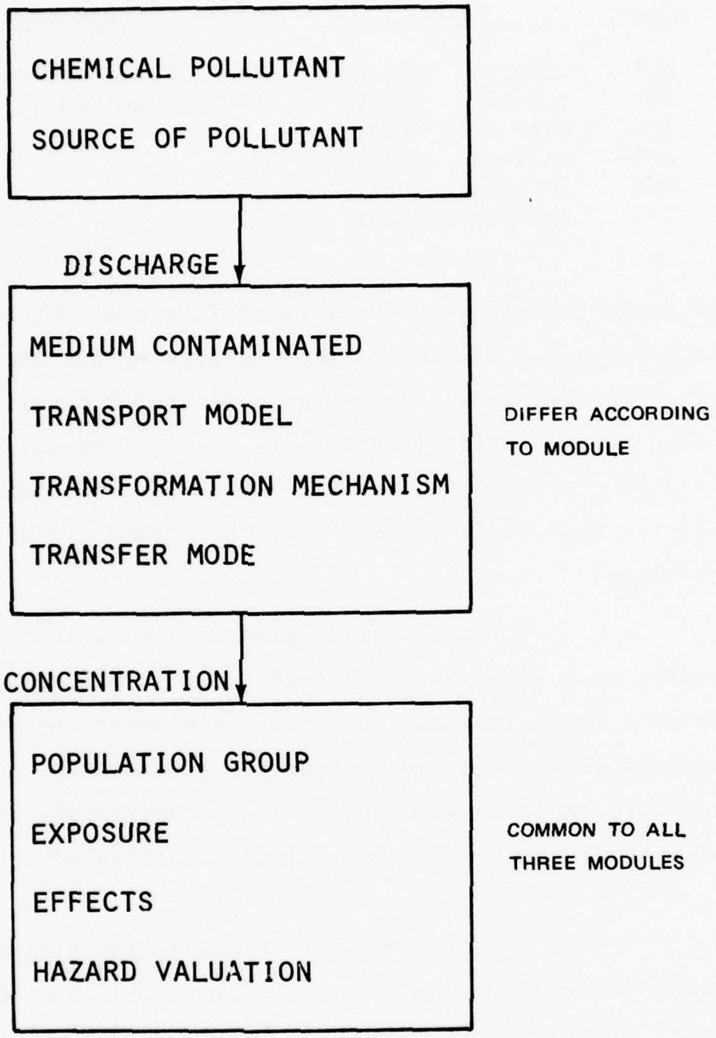

FIGURE A.3-1 OVERVIEW OF THE HAZARD ESTIMATING AND RANKING SYSTEM

Table A.3-2

LOCATIONS OF INTEREST
TO THE ARMY CHEMICAL PROJECT

Code	Army Installation Plants	Code	Installation Restoration
HOL	Holston (HAAP)	RMA	Rocky Mountain Arsenal (RMA)
JOL	Joliet (JAAP)	PBA	Pine Bluff (PBA)
ICY	Lake City (LCAAP)		
RAD	Radford (RAAP)		
SUN	Sunflower (SAAP)		
VOL	Volunteer (VAAP)		

and direction and atmospheric stability class by season of the year. In surface water, dilution of the effluent by average and low flows of affected river reaches is the basic transport model. Times of transit from source to population location are also estimated. In groundwater, a simple diffusion model for vertically-confined diffusion in a uniform-velocity flow field is used. Transit times are especially important in this model.

For munitions plants, a constant source term is assumed, leading to a steady-state solution for both air and water pollutants. For land contamination, an initial contaminating event is assumed, followed by decreasing inputs into the groundwater. Concentrations thus vary with the time after this event. Ordinarily 1974 is the time at which the concentration "snapshot" is estimated.

Transformation--Transformation refers to the chemical change of the pollutant under consideration to other compounds. Even though the products of the transformation may also be toxic, they are treated as no longer associated with the primary chemical, but instead are candidates for another exercise of the hazard system.

Transformation takes place during the transport process, so that for primary chemicals, the total inventory of material decreases with increasing transit time to reach the population-at-risk. For degradation products, the concentrations may actually be higher farther from the source, but the model does not presently provide for such detailed calculation.

All transformation processes (hydrolysis, oxidation, photolysis and photo-oxidation, and biodegradation) are assumed to take place with linear kinetics. Mathematically, the rate of decrease of the material present is assumed to be linearly related to the amount present at any time:

$$\frac{dq}{dt} = - \lambda q$$

In this equation, q is the quantity present and λ is a rate constant with units of $(\text{time})^{-1}$. It is likely that many of the transformation processes are nearly linear, for example, hydrolysis. However, it is known that the linear hypothesis does not work well for biodegradation. More complicated models, nevertheless, are not thought to be justified.

In air, a net rate constant (or half-life, $T_{1/2} = 0.693/\lambda$) can be inserted in the dispersion model, and the resultant concentration will be correspondingly reduced. However, transformation is not significant for the combinations of pollutants and receptor locations studied so far, owing to short transit times in comparison with the estimated half-lives.

In surface water, the exponential reduction in concentration for the travel time to a population at risk is calculated and applied to the transport-derived concentration. In groundwater, the diffusion constant is modified to take transformation into account, and the concentrations are correspondingly reduced.

Transfers--This component deals with transfers from one medium to another (evaporation, adsorption and precipitation, deposition, and percolation). For most Army chemicals studies so far, such transfers are more important in reducing the concentrations in the source medium than they are in increasing concentrations in the receiving medium, except for the land to groundwater transfer.

Linear kinetics are also assumed for the rates of transfer. In fact, the concentrations in air, surface water, and groundwater are computationally reduced simultaneously, using an overall rate constant incorporating both transfer and transformation rates.

Populations-at-risk--This part of the model simply describes the locations and numbers of the populations-at-risk to chemical pollutants of the various environmental media. Both human and nonhuman populations are included.

The units are commonly simple numbers (human population of a town or fish population of a reservoir) but can be other natural units (number of acres of crops in a region).

The population of an area is considered to be concentrated at a single point to describe its location most simply. There are two approaches to identifying these points. In the first approach, natural groupings of population are identified first, and then a point representing them is chosen. These points are then used as inputs to the transport models, and the corresponding concentrations are computed. Alternatively, an arbitrary grid of points can be specified as input to the transport model, and later the populations associated with one or more of these points can be estimated. In the first case, one risks the waste of identifying points with no significant exposure, and in the latter case, identifying points with no significant population. The first method has been chosen as conceptually the simplest.

The variety of populations-at-risk to pollutants in a given medium has been severely limited thus far. Most of this limitation has to do with the availability of data on effects. The possibility of describing subpopulations, such as male and female, old and young, susceptible and resistant, was limited on the one hand by limited knowledge of the variations in effects, and on the other by the data requirements on the size of these populations.

Exposure--The exposure model links the concentrations in environmental media as predicted by the transport, transformation, and transfer models to the determinants of the effects that are to be estimated.

A simple component of this model is the relationship of concentrations in raw source water to those in finished drinking water. The conversion factor is termed the treatment efficacy, and depends on the technology of the water treatment plant for the population-at-risk and on the characteristics of the pollutant.

A more conplex question is related to the determinants of effects. Most effects are dependent both on the rate of exposure to the chemical and the total exposure over a period of time. The route of exposure is also important.

Certain effects (most commonly acute effects) are dominated by the rate of exposure; these effects are characterized by strong recovery phenomena and in practice by relatively high thresholds. Although it is the actual exposure dose rate that is important, this rate is linearly related to the concentration in the medium of exposure, all other factors remaining constant. Consequently, effects data are usually expressed in terms of ambient concentrations, for example, LC_{50} (lethal concentrations in water for fish) or TLV (threshold limit value for inhalation).

Other effects (usually long-term) seem likely to be dominated by total exposure. In radiation, it has been demonstrated that cancer risk is nearly proportional to total dose over a wide range of doses. Many other cancer risks seem to be dominated by total exposure. Thresholds are more likely to be low or zero. Consequently, the proper determinant for such effects is some measure of total exposure, such as the total inhalation of a chemical over a year. Conversion of concentration to "dose" thus requires knowledge of breathing or drinking rates for air and water, respectively.

It is recognized that concentrations in air lead to dermal and oral (swallowing of mucous) exposure, as well as inhalation ones. Similarly, surface water can lead to dermal exposure for humans (bathing, swimming). Those exposures are currently thought to be secondary to the areas included.

Effects--The choice of which effects to consider and how to treat them is extremely difficult. The effects treated so far are shown in Table A.3-3.

Table A.3-3

TREATMENT OF EFFECTS

Effect	Code	Routes of Exposure	Exposure Determinant
Carcinogenicity in humans	C	Respiratory Oral	Dose Dose
Severe chronic effects in humans	CTG	Respiratory Oral	Dose Dose
Recoverable chronic effects in humans	CTR	Respiratory Oral	Dose* Dose*
Acute toxicity in humans	ATX	Respiratory Oral	Concentration Dose*
Acute toxicity in fish (fish kill)	FKL	Immersion (water)	Concentration
Chronic toxicity in fish	CFS	Immersion (water)	Concentration
Yield reduction in crops	CYL	Immersion (air)	Concentration

---

*Some of these effects may be concentration-dependent.

The key concept in modeling effects is what is ordinarily termed the dose-response relationship. This is the functional relationship between the exposure variable and the severity of the effect. Severity in some cases means the degree of illness for an individual at various levels. For example, headache at one part per million, nausea at three, convulsions at seven, and death at ten. However, the measure of severity used here is the percentage of an exposed population that incurs the effect at a given level of exposure. This percentage depends on the distribution of susceptibilities as well as on statistical phenomena such as the likelihood of one molecule of a chemical interacting with genetic material to produce a mutation.

It is assumed for simplicity, even in the face of conflicting evidence in many cases, that all dose-response relationships are linear with zero threshold, as shown in Figure A.3-2. This assumption is conservative for most pollutants, and puts all effects on an equal footing in terms of low-dose behavior. In an earlier version of the system, only cancer was assigned zero-threshold, and turned out to be the only effect with nonzero hazards. It is also assumed that exposures almost never reach levels at which all members of a population are affected. However, the model limits the percentage affected to be less than or equal to 100%. Exposure can be given either in terms of total dose (as illustrated) or in terms of concentration. The important parameter is the slope of the linear relationship.

Two of the properties of the linear no-threshold dose-response relationship are also illustrated in Figure A.3-2. At the top of the figure, it is shown that for a given dose to every member of a population, the same percentage of the population is affected regardless of the size of the population. At the bottom of the figure, if a given amount of material is divided in any way among any number of individuals, the _same number of affected individuals is expected_.* This second property allows us to be less precise in distinguishing among population groups exposed at different levels.

There are two different possible philosophies for treating effects in the event of missing data.

- Assume that the effect is not important for this chemical.
- Assume that the effect might be important. Assign a default value for the slope and estimate uncertainty.

Because of an existing methodology for estimating the slopes for carcinogenicity (Dean and Helmes, 1974), the latter philosophy

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*Within limits. If any individual receives more than the 100% dose (333 mg in this example), the number of effects declines.

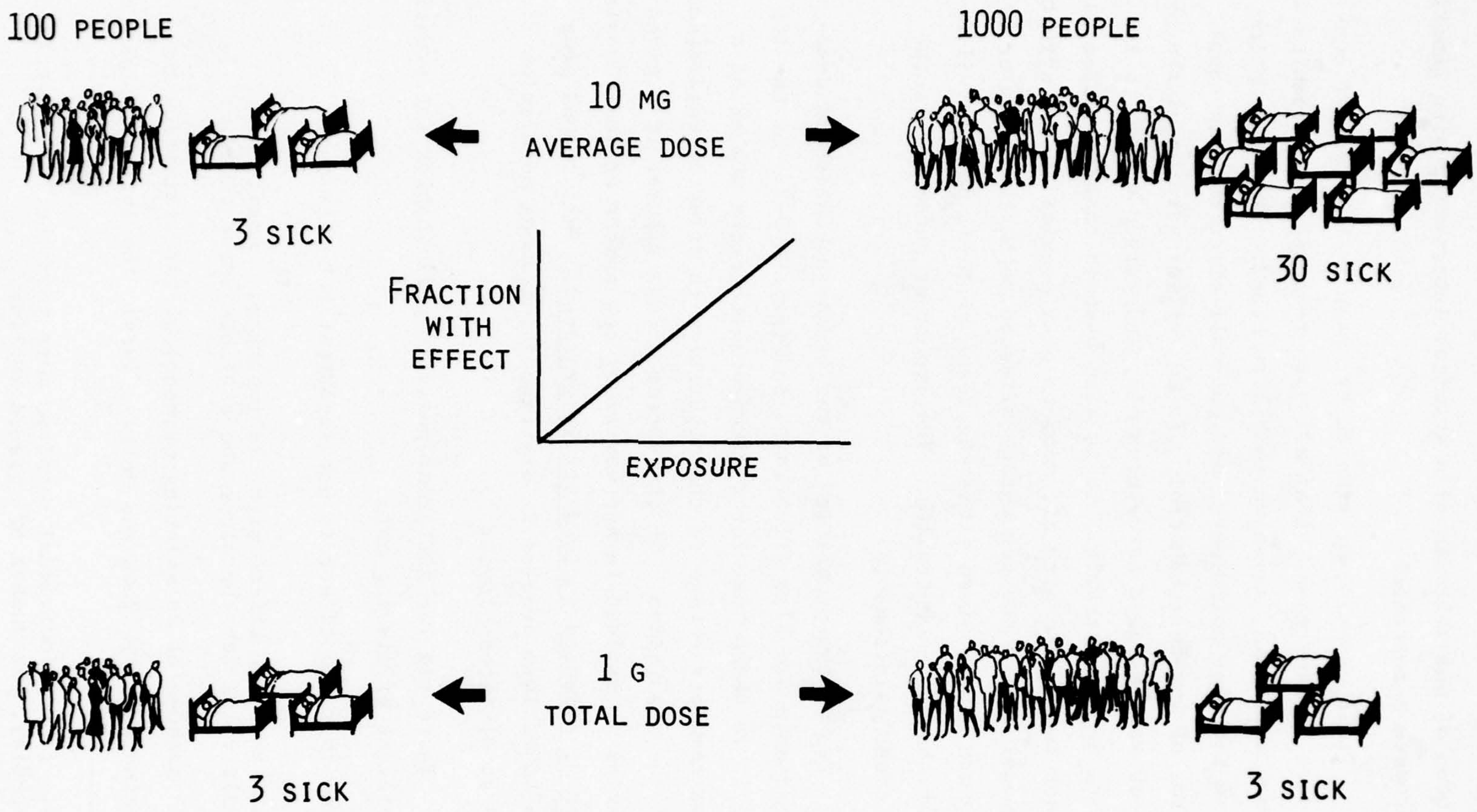

FIGURE A.3-2 LINEAR NO-THRESHOLD DOSE-RESPONSE RELATIONSHIPS has been adopted for this effect. So far, the former philosophy has been used for many of the other effects. It is probably more correct for allocating research funds to use the latter philosophy throughout, and it has been implemented for the other chronic human effects.

The actual number of effects is computed by multiplying the percentage response and the number of individuals in the population-at-risk. The result is usually expressed in terms of the number of new cases each year.

Valuation--The final model of the hazard ranking system is valuation. A system of values for each of the effects allows the hazards from the various effects of the different chemicals to be intercompared. All that is required is to assign a relative value to each effect, choosing a nominal value for one of them.

However, for other purposes, it is useful to have the values expressed in concrete units. Accordingly, the values have been expressed in monetary terms: the dollar value of one case of each effect. In the case of crop losses, the economic impact is relatively straightforward: values for a loss on one acre's production of cropland can be obtained by estimating yield per acre and dollar value of yield for several important crops and then averaging them (Bureau of the Census, 1974b). For fish kills, the value can be estimated from both the commercial fishing value and the sports-fishing recreational values (Jurgens, 1975). For illness, both economic measures (worktime loss, physicians' and hospital costs) and human suffering contribute to the value. The valuation of human life is even more difficult to set. However, the problem has been addressed (Moll et al., 1975). A working set of values if shown in Table A.3-4. It is also possible to assign subjectively determined relative values to the effects and then scale them to one established number (Brown et al., 1976). However, the subjective ratios do not seem to be transitive--the ratio of values for death and a cold does not seem to equal the ratio of values for death and emphysema times the ratio of values for emphysema and a cold.

Summary--The hazard estimating and ranking system thus consists of a comprehensive mathematical model of the pollution process

Table A.3-4

VALUATION OF EFFECTS

Code	Effect	Units	Value/Unit	Range
C	Human cancer	Cases	$300,000	$100,000-500,000
ATX	Acute toxicity (death)	Cases	200,000	100,000-400,000
CTG	Serious chronic toxicity	Cases	300,000	100,000-400,000
CTR	Recoverable chronic toxicity	Cases	30,000	10,000-100,000
FKL	Fish kill	Fish	1	0.2-5
CFS	Chronic fish toxicity	Fish	1	0.2-5
CYL	Crop yield loss	m^2	0.03	0.01-0.15

that expresses hazards as the annual dollar values of effects caused by various pollutants discharged from various Army activities and affecting various population groups through several environmental media. Figure A.3-3 shows a conceptual diagram of the major modules of the system (for air pollutants, water pollutants, and groundwater contaminants) and of the important components of each module.

As explained in Section A.2.4.1, the hazards can be computed in disaggregated form at the six-subscript level of detail. They can then be aggregated in any desired fashion. One particularly useful aggregation sums all hazards attributable to a given chemical. These aggregated one-subscript (i) hazards can be ordered on the value of the hazard to produce a ranked list of chemicals. This hazard-ranking is useful in determining which chemicals may be the Army's biggest problems, although by itself gives no information on preferred research programs. It can also be compared with selected values for hazards of civilian chemicals, estimated in a similar fashion, for putting the Army's chemical problems into perspective.

To assist in the choice of civilian chemicals for comparison with Army chemicals, a previous SRI study for the National Science Foundation was used (SRI, 1975). This study compiled data relevant to the environmental effects of 80 synthetic organic chemicals. A menu

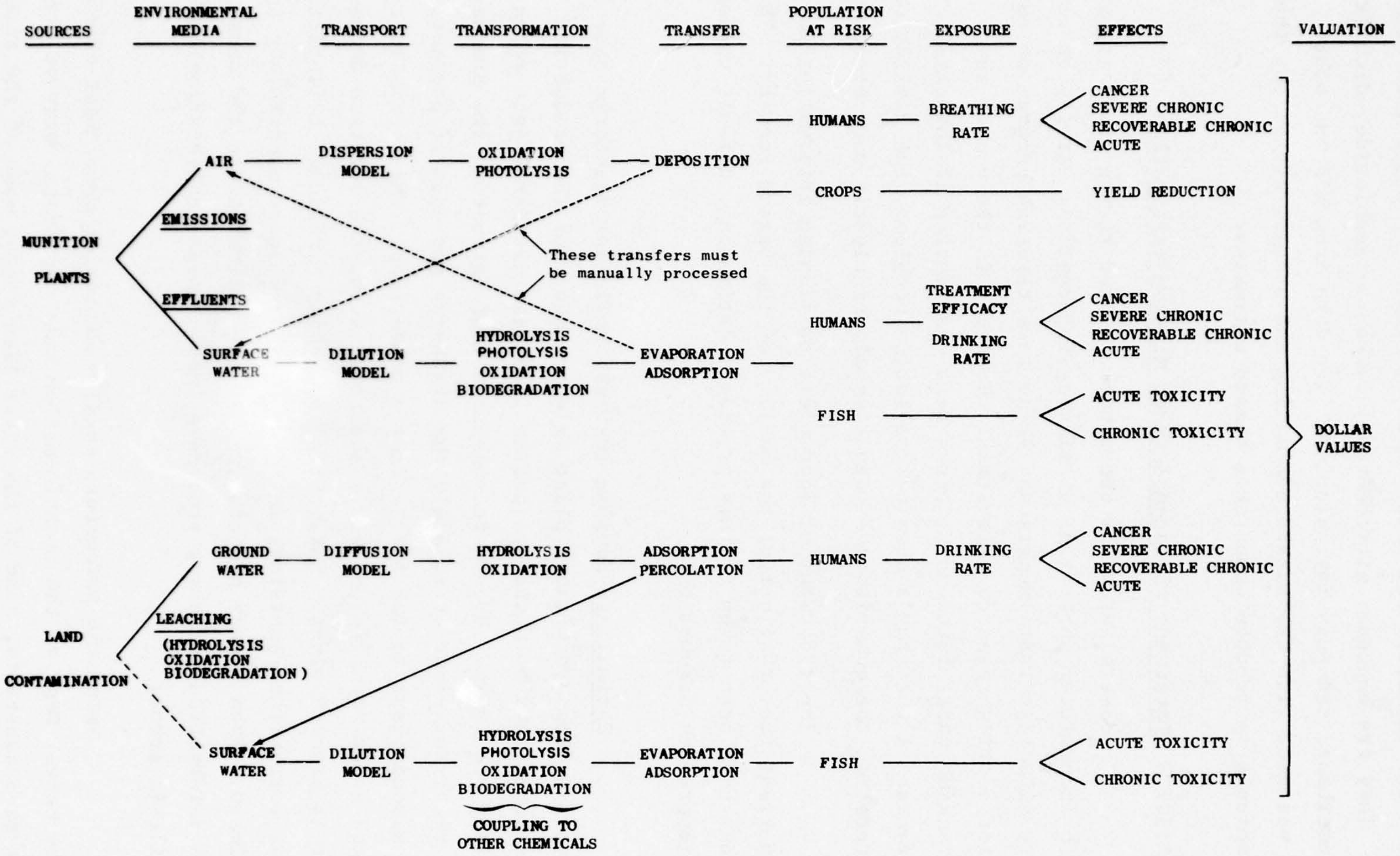

FIGURE A.3-3 OUTLINE OF THE HAZARD ESTIMATING AND RANKING SYSTEM of 10 civilian chemicals was recommended to EPRD, from which five were chosen. They are benzene, nitrobenzene, carbon tetrachloride, dichlorodifluoromethane, and polyvinylchloride. The data from NSF and other sources was used with the hazard estimating and ranking system for the Army chemicals to produce comparable hazard estimates.

A.3.1.3 Treatment of Incomplete or Missing Information

Several sections above have alluded to the necessity to deal with incomplete, uncertain, or missing information. It is, of course, this very situation that imparts any value to a research program or to a system for setting research priorities. However, in the use of the hazard-ranking part of the methodology as a description of the extent and character of the Army's chemical pollution problems, the limitations in interpreting the quantitative output should be clearly understood.

The treatment of incomplete or missing information is the most important factor affecting the quality of the hazard ranking. Three approaches have been taken to this problem: estimating, default values, and no-importance assumptions.

Estimating--Suppose that the pollutant discharge rate for nitroglycerin from a munitions plant is not known, but the production level is known, and both the production level and discharge rate at another plant are known. Then a reasonable way of estimating the discharge rate at the first plant is to apply the discharge per unit of production for the second plant to the first plant's production. This estimate can be changed up or down, if one knows something about the relative degree of controls at each plant. Estimating, by having a rational scientific basis, is better than guessing, in terms of having lower uncertainty in the estimate. Even "hard" numbers are usually estimates, in the sense that the information-gathering procedure (measurement, calculation) has some built-in error.

Among the parameters usually estimated are: most of the discharge rates, many of the transformation rate constants, many of the transfer rate constants, some of the river flow rates, most of the fish populations, most of the agricultural populations, some of the water treatment efficacies, all of the carcinogenic dose-response slopes, some of the other toxic properties, and all of the effect values.

Default Values--Default values are estimates without as firm a basis. If one has little or no basis for a given estimate, then he can supply a default value. A default value can be an ordinary, typical modal, or average value found for a sample of measured values. For example, suppose nothing is known about the solubility of a chemical in water. But solubilities of other compounds have been measured, and have been found to vary from miscible (soluble in all proportions) to insoluble (solubilities of one hundred parts per million or less). Only a few seem to be soluble (50,000 ppm) or very soluble (500,000 ppm). Therefore, it seems reasonable to choose a default value of 1,000 ppm, corresponding to slightly soluble.

Other properties that often require default values are: vapor pressure and the corresponding estimates of evaporation rates, rate of transfer to soil or sediments, other transfer rates (or half-lives), some of the transformation rates, particularly for biodegradation, most of the treatment efficacies, and some of the discharge rates, particularly for land contaminants.

No-importance Assumptions--A final treatment, usually used as a last resort, is to assume that missing information implies that the phenomenon in question is unimportant. This technique applies mainly to branches of the methodology that were simply never developed at all: ecosystem disturbance, for example. However, there are also individual data elements that are treated as unimportant when data are missing. Many of the toxicological parameters fall in this category. For example, if no data for phytotoxicity to crops have been reported for a given chemical, crop yield loss is assumed to be unimportant. Another major area where this treatment is used is the pollutant discharge rates: if no discharges from any plant have been reported, it is generally assumed that none exist. Some of the intermedia transfers and some of the transformation possibilities are assumed to be unimportant. Effects beyond arbitrary boundaries for air pollution and water pollution from munitions plants are ignored.

A.3.1.4 Implementation

Implementation of the hazard ranking system consists of two major stages: data acquisition and data processing. Data processing is a combination of manual preprocessing to standard data formats, followed by computer processing of prepared data.

Data Acquisition--Data acquisition is by far the more difficult of the two stages. In one sense, there is a surfeit of data; scores of Army reports and hundreds of scientific documents have information relevant to the hazard system. The first requirement for an economical hazard system is to select those sources in which the data are most concentrated: handbooks, lists, review articles, problem assessment reports. But even with such a start, the data are usually not in the form desired, and a great deal of preprocessing is necessary. Especially time consuming is the development of estimates for required data elements from more basic quantities.

Data acquisition is usually divided up according to the system module under consideration, and is done for a group of chemicals in parallel. However, when a new chemical is added, all the data elements for it must be developed in series. The sources and procedures for data acquisition and preprocessing are described in detail for each module in Annex A.B.

Data Sheets--Once the required input data elements are acquired, they are entered on a set of data sheets. The data sheets are designed to all have the same general format and to be given directly to a keypunch operator for preparation of computer input cards. The general format of the data sheets is shown in Figure A.3-4. The variable for which a given card applies is shown in the first 3 columns. Here, for example, one could enter "S" for the slope of the dose-response relation. The next 18 columns accept up to six subscripts that describe the hazard(s) to which the variable is input. The value of the variable, appropriate units, and the uncertainty in the value are given next. (The computer checks that the units are appropriate for the variable in question and

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units								Uncertainty Codes			Documentation	Continued
																+ or −		b or %		
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.3-4 AMRDC POLLUTANT HAZARD MODEL DATA SHEETS converts them to standard CGS units for computation.) The documentation field accepts any textual statement the operator wishes to enter, and can be continued on up to three additional cards by marking column 72. Documentation ordinarily includes the source and date of the data--often the name of the operator. Finally, a "case code" is attached to each record to distinguish between one operation of the hazard estimating and ranking system and another, for example, between a civilian and a military run or between a 1976 and a 1977 run.

There are currently 13 different program input forms generated from the basic format, divided into nine classes. These are shown in Table A.3-4; they are distinguished both by the subject matter of the data to be entered and by the specific subscripts that must be supplied for each variable. The exact meaning of the terms used in Table A.3-5 will become apparent in the next three sections. Illustrations of the specific forms and instructions for their use appear in Annexes A.B and A.C.

Table A.3-5

CLASSES OF PROGRAM INPUTS

I	Effects, Population Types, Locations, and Chemicals
II	Populations
III	Valuation of Effects
IV	Slope, Threshold, and Dose-to-Concentration Ratios
V	Emission/Effluent Rates
VI	Air Pollutant Model--Concentration Multipliers
VII-A	Water Pollutant Model--Flow Rates and Transit Times
VII-B	Water Pollutant Model--Transformation - Transfer Rate
VII-C	Water Pollutant Model--Purification Factors
VIII-A	Groundwater Pollutant Model--Diffusion Constants and Flow Rates
VIII-B	Groundwater Pollutant Model--Locations of Wells and Groundwater Outfalls
VIII-C	Groundwater Pollutant Model--Transmissivity, Gradient, and Length of Groundwater Outfalls.
IX	Concentrations

Computer Implementation--A hazard estimation computer program called HERS (for Hazard Ranking and Estimating System) has been designed to accept cards generated from the data sheets and produce a synopsis of hazard estimates at various levels of aggregation. Details of inputs and outputs, logic, and program listings appear in Annex A.C.

Basically, the computer accepts data cards in (almost) any sequence and then checks, sorts, and stores the data in a convenient form. It then computes six-digit hazards in a systematic fashion and aggregates them by chemical, i, and by location of Army activity, j. An intermediate output of the program is a detail of six-subscript hazards, as shown in Figure A.3-5, which includes a processed summary of input data. The final output is a matrix of hazards by chemical and location, with both row and column sums. A sample of this output is shown in Figure A.3-6. (Warning: Both of these illustrations were developed with dummy data and do not represent final hazard estimates.)

The computer also prints out, on command, extensive diagnostic statements for missing or erroneous data. This printout is especially useful in locating a datum omitted by oversight.

The hazard totals can then be sorted by hand to create a ranked list by either chemical or location, to satisfy the intermediate (Task 1) project objectives.

A.3.2 Common Elements Among the Three Major Modules

Significant common features exist among the three (air, water, groundwater) major modules of the hazard estimating and ranking system. For convenience, they are discussed here rather than in the sections detailing each module.

A.3.2.1 Basic Hazard Formula

The most general expression for a six-subscript hazard is

$$H_{ijmnk\ell} = V_{n\ell} \, N_{jmnk} \, S_{im\ell} \, b_{im\ell} \, C_{ijmnk\ell}$$

```
                POP SUB      HAZARD  -----------------VALUES IN CGS UNITS------------------
CHM LOC MED TYP LOC EFF  $/YEAR     DOSE      POP        V          S        SMB       B
--- --- --- --- --- --- ------   -------- -------- ---------- -------- -------- -------.
TNT HOL H2O HUM   1 C    4394.   .320E-10 .290E+05 .300E+06 .500E-03 .158E-01 0.
TNT HOL H2O HUM   2 C    7411.   .730E-11 .214E+06 .300E+06 .500E-03 .158E-01 0.
TNT HOL H2O HUM   3 C      65.   .120E-11 .114E+05 .300E+06 .500E-03 .158E-01 0.
TNT HOL H2O HUM   4 C      16.   .525E-12 .659E+04 .300E+06 .500E-03 .158E-01 0.
TNT HOL H2O HUM   5 C       4.   .822E-13 .108E+05 .300E+06 .500E-03 .158E-01 0.
MNT VOL AIR HUM   1 C     267.   .627E-10 .900E+03 .300E+06 .500E-03 .231E+03 0.
MNT VOL AIR HUM   2 C      53.   .279E-10 .400E+03 .300E+06 .500E-03 .231E+03 0.
MNT RAD AIR HUM   3 C      92.   .110E-10 .177E+04 .300E+06 .500E-03 .231E+03 0.
```

FIGURE A.3-5 SAMPLE SIX-SUBSCRIPT HAZARD OUTPUT OF HERS

```
HAZARD SUMMARIES BY CHEMICAL AND LOCATION

CHEMICAL          HOLSTON       JOLIET      NEWPORT      RADFORD   VOLUNTEER    ALL LOCS

SODIUM CHLOR         0.00         0.00         0.00         0.00        0.00        0.00
  ATE OR CHLOR
  ATE SALTS

MONONITROTOL         0.00         0.00         0.00        91.97      319.75      411.71
  UENES

2.4.6 TRINIT     11890.69         0.00         0.00         0.00        0.00    11890.69
  ROTOLUENE

ALL CHEMS        11890.69         0.00         0.00        91.97      319.75    12302.40
```

FIGURE A.3-6 SAMPLE HAZARD MATRIX OUTPUT OF HERS where

H	is the hazard in dollars/yr.
$V_{n\ell}$	is the value of an effect ℓ in population type n, in dollars per case.*
N_{jmnk}	is the number of individuals* in a specified group k of population type n associated with medium m at location j.
$S_{im\ell}$	is the slope of the exposure-response relationahip for effect ℓ from chemical i in medium m, in units of fraction of exposed population per unit of exposure dose* (specification of the subscript ℓ also specifies the population at risk, n, since values $V_{n\ell}$ are specified only for appropriate combinations of n and ℓ--for example, no fish kill effect is specified for human populations).
$b_{im\ell}$	is the dose-to-concentration ratio for effect ℓ from chemical i through medium m, in appropriate units (for example, if dose in grams is the unit of exposure, then $b_{im\ell}$ converts concentration units to annual dose in grams).
C_{ijmnk}	is the concentration of chemical i produced at group k of population type n by discharges at location j into medium m, in appropriate concentration units.

To illustrate, suppose the concentration C[†] were estimated to be 10 mg/liter of water, and the effect was related to total dose rather than to concentration. Then for a human population, we would use b = 500 ℓ/yr, the typical drinking rate. This would give a dose of 5,000 mg/yr or, converting, 5 g/yr. Suppose the slope of the dose-response relationship extrapolated to 100% (fraction = 1) at 10^4 g exposure dose. Then $S = 10^{-4}\ g^{-1}$, and the expected incidence rate would be 5×10^{-4} $(yr)^{-1}$. If this occurred in a population of N = 20,000 people, then the expected number of cases would be $2 \times 10^4 \times 5 \times 10^{-4} = 10$ cases/yr. If the value per case were \$100,000, then the hazard would be \$1,000,000/yr.

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[*] Or other appropriate unit.

[†] Subscripts are dropped here for brevity

A.3.2.2 Concentration Estimates

The above formula applies to all three media, assuming

- Appropriate effects, populations, locations, chemicals, and media are selected, and
- Appropriate concentrations can be estimated.

The concentrations to be used are those appropriate to the effect under consideration. For example, total-dose effects are related more to the average concentration over a year than to a peak concentration, but acute toxic effects are often related to the peak concentrations, for example, fish kills during low-flow conditions in rivers.

When concentrations can be measured over a time adequate for averaging, the experimental results are probably most accurate for expressing the concentration. However, concentrations can also be estimated from a model of pollutant transport, transformation, and transfer from more fundamental data. The hazard estimating and ranking system provides for either direct input of a concentration or its calculation from one of the medium-specific modules. Moreover, the direct concentration input feature can be used when concentrations are generated by a model that is subsidiary to and outside the basic hazard system. This situation is virtually true for the air pollution module, in which concentration multipliers are estimated by an external model.

A.3.3 Conceptual Limitations

The quality of the research allocation methodology depends on how well the hazard estimation system can treat the reduction in hazard uncertainty attributable to a given research program. Thus, the estimation system should ideally treat all phenomena important to the final hazard estimate. Unfortunately, there are major conceptual limitations to this ideal.

There are two important types of conceptual limitations to a fully satisfactory system for estimating hazards. The first type of limitation results from the existence of phenomena that no one recognizes as being important. For example, before the chemical basis of heredity was discovered, the concept of chemically-induced mutations was not possible, and no one would have thought of putting a mutagenesis model in his hazard system. The unpredictable is unpredictable; it justifies some allocation to basic research.

The second type of conceptual limitation includes phenomena that are known and could be important. The principal limitation here is that the phenomena are poorly understood and difficult to treat quantitatively, and that even the hazard ranking system must put emphasis on the areas of most potential payoff, namely, those that are known to be important. Even when a phenomenon is known to be important, however, a secondary limitation, lack of information, can come into play.

A.3.3.1 Limitations in Effects Considered

The variety of possible biological effects and species affected from chemical exposures is bewildering. There are differences of severity (death, serious illness, minor illness, annoyance, subclinical manifestations), of time scale (acute, subacute, chronic, delayed), of kind (respiratory illness, central nervous system disturbance, dermatitis), and of specificity (species-specific, ecosystem disturbance). This variety cannot be completely, or even moderately well covered by a modest system. Consequently, it is necessary to select a set of effects that will be systematically addressed and to disregard the others unless they stand out.

A.3.3.2 Limitations in Environmental Pathways Considered

Just as there are many effects to consider, the phenomena affecting the pathway of chemicals from source to population at risk are many. These phenomena include media of introduction, physical intermedia transfers, transport within media, chemical and biological degradation (which result in new chamical pollutants), biological pathways, and mechanism of exposure. Many of these phenomena have been grossly treated in the system; but there are severe data limitations to specific treatment.

A.3.3.3 Limitations in Sources Considered

One particularly difficult conceptual problem is what to do about munitions plants that are either inactive or operating at well below capacity. The discharges from operating plants are, at best, known for 1972-1973 production levels. Discharges at capacity would generally be presumed to be higher, but probably not linearly so, and in some cases possibly lower.

At the installations with land contamination, the conceptual limitations are concerned with two questions: whether on-site or off-site problems are of most concern and whether current or future problems should be emphasized.

All of the contaminated installations may be causing problems off site as well as on site. For example, concentrations of DIMP, DCPD, and chlorates have been found outside the boundaries of Rocky Mountain Arsenal (RMA) in ground and surface water. As long as the installation itself is under Army control, the off-site problems are of most concern to EPRD. However, many of these installations are candidates for restoration before return to civilian uses. Thus, research concern is beginning to focus on the future on-site exposure of civilian populations to future concentrations of pollutants. This situation is especially complicated by the need to make assumptions about

- Degree of cleanup achieved
- Size of populations at risk
- Behavior of the populations.

Currently, the research is focusing on off-site problems.

The question of future versus present problems has two aspects. The first is closely associated with the off-site/on-site question, because on-site problems are principally of future concern. The second aspect is that the pollution from land contamination is assumed to be dynamic, in contrast with that from munitions plants, which is assumed to be in a more or less static equilibrium. Specifically, the movement of contaminants is a slow process, and the pulse of concentration is gradually moving further and further off site. Since the populations-at-risk tend to be larger the farther from the installation boundary, future problems could easily be more severe than present ones. On the other hand, the pollutants are gradually degrading, depositing, and diffusing, so that there is a strong likelihood that future hazards will be lower.

Currently, off-site hazards are calculated for the present (usually with 1974 data). However, the sensitivity to the time variation could be tested by selecting a future time and repeating the hazard calculation. For RMA, a time around 1987, when the Shell lease expires, seems a reasonable test frame.

A.3.3.4 Limitations in Chemicals Considered

Hundreds of chemicals have been proposed as possible components of munitions plant discharges or residual contaminants of installations. These include raw materials, manufactured products, by-products, wastes, and breakdown products of the primary chemicals. Many have been nonquantitatively identified in waste streams or environmental media, and some have been quantitatively assayed.

A.3.3.5 Availability of Information

As intimated several times earlier, one of the most serious conceptual difficulties is the lack of solid information for making hazard estimates. This lack falls into two major categories: models and data.

Models--The entire hazard estimating and ranking system is a mathematical model of the processes leading from the chemical pollution of the environment to the eventual biological effects and their valuation. It consists of a large set of submodels, each treating some phenomenon of natural. However, nature is complicated and most mathematical models must, for practical reasons, be simple. Consequently, the models do not always simulate nature well. Furthermore, scientific knowledge about (or even of!) these natural phenomena is incomplete; in many cases the processes are not understood well enough to even begin a mathematical treatment. Only those processes reasonably well understood are included in the system.

Data--Even when a good model is available, it may be based on measurements made on only a few chemicals. The vast majority of Army chemicals is unlikely to be on this select list. Thus, lack of data about a particular compound seriously limits its hazard estimation. In many cases, data are so sparse that even when the process is understood, it is not worth including in the system. However, the mere fact that data are missing or models unavailable already suggests attractive areas for further research.

A.3.3.6 Amenability to Research

A final conceptual problem concerns the degree of detail desired in the hazard system models. For example, the estimate of fish populations at risk to water pollutants could be built up from data on species diversity, population dynamics, predator-prey relationships, food availability, sports and commercial fish catches, stocking of reservoirs, and so on. However, most of these are beyond the research interests of EPRD, and some of them are not very amenable to research. Since it is unlikely that EPRD would want to devote research resources to reducing the uncertainty in the fish populations at risk, it is better to put in the estimated population directly rather than to build it up from more fundamental information.

A.4 AIR POLLUTANTS FROM MUNITIONS PLANTS

This section is the first describing the major modules of the hazard estimating and ranking system. Many of the detailed procedures are relegated to Annex A.B for the use of specialists. The section is organized according to the components shown in Figure A.3.1.

A.4.1 Sources

The first four air pollutants listed in Table A.4-1 are discharged to the atmosphere during manufacture of TNT, nitroglycerin, RDX, HMX, and other explosives and intermediates, and their known discharges are shown. The last three pollutants are associated with civilian activities as well as Army ones, and are assumed to be covered by civilian standards.

The characteristics of each source include: the discharge rate, the equivalent stack height (some sources are fugitive, rather than being emitted from a stack), the stack diameter, and the stack gas temperature and velocity. These data elements are described further in Section A.4.2 below, and their values are listed in Annex A.C.3.1 for the SRI Version of the Climatological Dispersion Model.

So far, only emissions from the Holston, Joliet, Radford, and Volunteer Army Ammunition plants have been included in this study. In some cases, different chemicals are emitted from different places in the same plant location complex. In such cases, it may be necessary to distinguish concentration multipliers for different chemicals at the same receptor location.

A.4.2 Transport, Transformation, and Transfer

Generally speaking, atmospheric transport is the phenomenon of most importance for air pollutants. Transformation of the pollutants to other chemical forms and deposition of the pollutants on land and water are processes that limit the long-term buildup of the pollutants in the atmosphere,

Table A.4-1

MAJOR AIR POLLUTANTS

Pollutant	Code	Estimated Waste at 40% Capacity (lb/day)	Plant	Remarks
Methyl nitrate	MN	990	HAAP	From RDX/HMX production
Tetranitromethane	TNM	369	VAAP	From TNT production
		1,300	RAAP	From TNT production
		?	JAAP	From TNT production
Nitromethane	NM	39	HAAP	From RDX/HMX production
Mononitrotoluenes	MNT	?		From TNT production*
Acetic acid		2,582	HAAP	Raw material used in RDX/HMX production
Acetic anhydride		48	HAAP	Raw material used in RDX/HMX production
Nitrous oxide		8,300	HAAP	From RDX/HMX production

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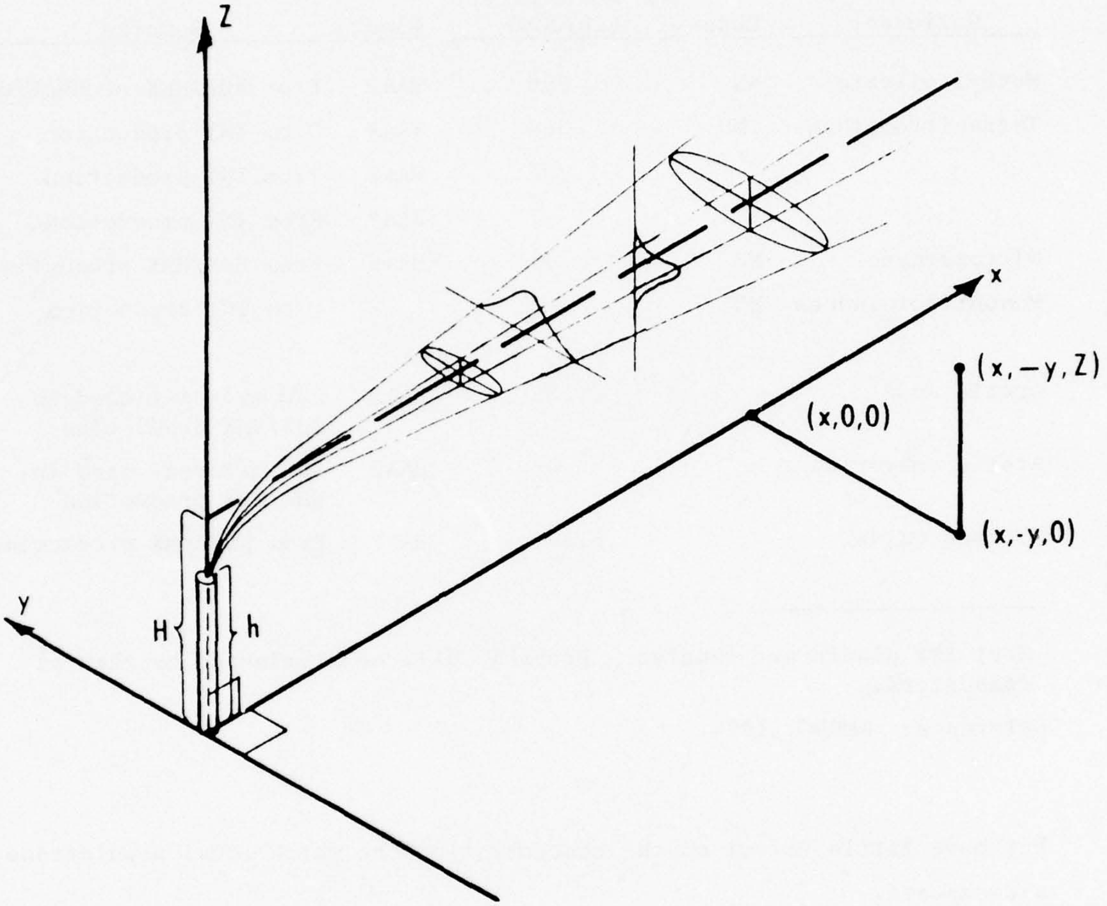
*Most TNT plants not sampled, Probably will be eliminated by thermal combustors.

Reference: AMRDC, 1974.

but have little effect on the concentrations to which local populations are exposed.

A.4.2.1 The Climatological Dispersion Model

Transport is estimated by the Climatological Dispersion Model used by the Environmental Protection Agency (EPA, 1973). This model accepts frequency distributions of winds by direction, speed, and atmosphere stability class; locations and characteristics of sources and receptor locations; and emission rates (g/sec) and chemical half-lives (sec). It then computes average concentrations ($\mu g/m^3$) at the receptor locations by a Gaussian dispersion model (Figure A.4-1). SRI has modified



Source: CDM

FIGURE A.4-1 COORDINATE SYSTEM SHOWING GAUSSIAN DISTRIBUTIONS IN THE HORIZONTAL AND VERTICAL the model to compute an annual average over four seasonal distributions, and has incorporated certain other changes in output formatting (see Annex A.C.3.1).

The model is currently used with unit emission rates to produce a concentration multiplier $[(\mu g/m^3)/(g/sec)]$ to apply to potentially varying emission rates. These concentration multipliers are computed for an assumed infinite half-life for the chemicals.

A.4.2.2 Transformation and Transfer Assumptions

Transformation is currently assumed to be unimportant for calculating concentrations. All half-lives for the four chemicals with respect to oxidation and photoinduced changes are probably much longer than the transit times to the receptor locations of interest, which are of the order of a few hours for the most prevalent winds. However, for possible future use the half-lives of the chemicals toward oxidation and photolysis have been estimated, and tend to be of the order of a few months to a year.

Transfer rates have not been estimated and are assumed to be small with respect to transit times. However, none of the pollutants are gases at ambient temperatures, and therefore they could condense on particulate matter and be deposited.

A.4.2.3 Output of CDM

Average concentrations over a year are computed on the assumption that the most important human effects are more dependent on total dose than on dose rate. This may make the computation of crop effects less accurate, since only growing-season concentrations should be used. However, there are few data on crop effects of these pollutants as yet. The average concentrations are known to be very sensitive to the choice of receptor locations, because of vagaries in the wind pattern. However, when several receptor locations are aggregated in the computation of a total hazard for a given chemical and location, there is a tendency for one location's hazard-uncertainty to cancel another's, and the uncertainty in the aggregate hazard is correspondingly reduced.

In the computation of average concentrations, one kilogram per year is about 3×10^{-5} g/sec. Other details of the transport module are given in Annex A.C.3.1.

A.4.3 Exposure

Exposure for crops is assumed to be measured by the average annual concentration. Thus, the exposure multiplier b is unity. Annual exposures for humans for dose-related effects, such as carcinogenicity, are computed by multiplying the concentration by the annual breathing rate, taken as 7,300 m^3/year. This rate is based on a rate of about 20 liters/minute during 8 hours of work and 10 liters/minute for the remaining 16 hours each day. It is also based on the total tidal volume of air inhaled, and probably overestimates the retained fraction. However, effects are probably expressed in terms of this total exposure rather than in terms of actual intake.

A.4.4 Populations-at-Risk

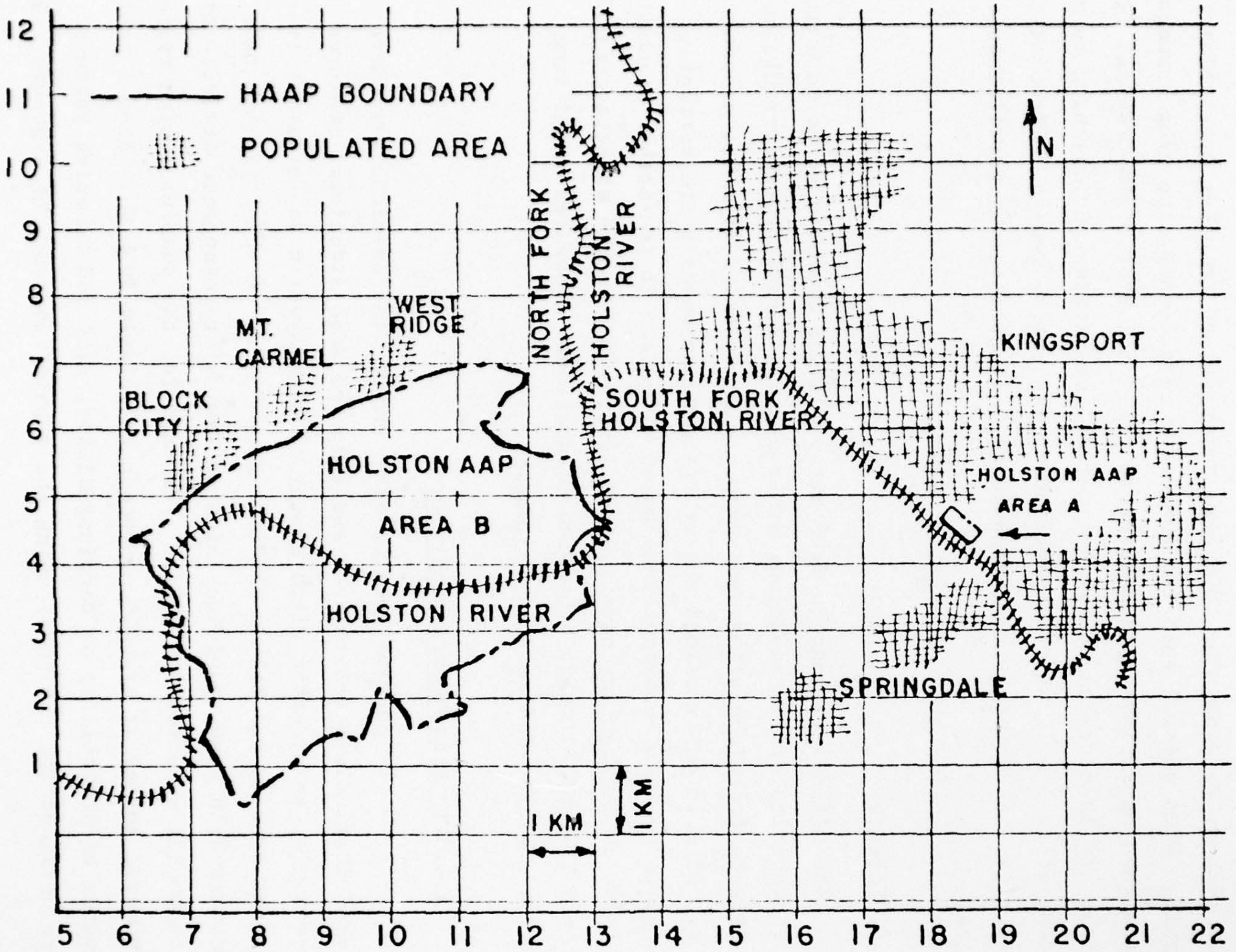
As indicated earlier, only humans and crops are assumed to be at risk from munitions plant air pollutants.

A.4.4.1 Humans

All significant population concentrations in the vicinity (about 30 km) of the sources should be identified. If winds are known to prevail in one quadrant, more emphasis should be placed there. Coordinates are established (on USGS topographic maps) for the sources and population centers, and the populations are determined from Census publications, road maps, or commercial atlases (Rand-McNally, 1973). Towns or portions of towns (such as census tracts) are the suggested level of aggregation (see Figure A.4-2).

A.4.4.2 Crops

Crop acreage for counties is available in the U.S. Census of Agriculture (Census, 1972). Total county acreage in crops is shown,



SOURCE: Mura, et al. 1974.

FIGURE A.4-2 RELATION OF THE HOLSTON ARMY AMMUNITION PLANT TO ADJACENT POPULATION CENTERS as well as that for individual crops. The acreage assumed to be of interest is that for all crops excluding hay crops.* This total crop acreage (excluding hay) is then assigned to general regions surrounding the munitions plants, by examining USGS maps for cropland or other open, flat terrain. When several such regions occur in a county, the crop acreage is assigned approximately according to the total area of the region. The regions are then associated with a set of coordinates for matching to a concentration level, which is applied to the entire region. Often it is impractical to estimate crop exposure at a finer level of detail than a county.

A.4.5 Effects

The effects of concern from air pollution are assumed to be human carcinogenicity from inhalation, other chronic severe or recoverable human effects from inhalation, and crop yield reduction from air concentrations. Effects on livestock and other nonhuman animals are currently assumed to be less important than human effects. It is further assumed that peak concentrations have reached levels where acute effects could be observed if they existed; otherwise occupational exposures would long since have caused controls to be imposed.

A.4.5.1 Human Carcinogenicity

If no experimental data exist, the chemical structure for each chemical is determined, and compared with structural features (for example, an aromatic nitro group) as displayed in an "activity tree" developed by Dehn and Helmes (1974). Each "node" of this tree has been associated with some suspicion, high or low, of carcinogenic activity of the compounds associated with it. For example, the suspicion with respect to aromatic amines or arsenic compounds is relatively high. From a table, estimates of probability of carcinogenicity, p(C) and relative potency, P, are obtained for the node, using the inhalation route of exposure. If

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* Hay crops are ordinarily of much lower value per unit area than other crops.

the specific compound has been discussed as carcinogenic (or noncarcinogenic), an upward (or downward) adjustment in p(C) is made. Then the slope of the carcinogenicity dose-response relationship is computed as:

$$S = 5 \times 10^{-4} \times p(C) \times P$$

where the constant is a scaling factor to place the units in fractional incidence per gram of exposure.

A.4.5.2 Other Chronic Human Effects

Few data are available on chronic human effects of the four principal air pollutants. Consequently, default values for severe chronic effects and for recoverable chronic effects have been used in initial tests of the hazard system (see Annex A.B.5.1).

A.4.5.3 Crop Yield Loss

It is known that certain pollutants, especially acid mists like sulfuric acid and acid sulfates, can severely reduce crop yields. Thus, there is room in the system for predicting such effects. However, no data on crop yield loss were found for the four pollutants.

A.4.6 Valuation

The values of interest so far are those for the above effects. The value of $300,000 per case for cancer is adopted on the assumption that most cancers from inhaled or ingested carcinogens are fatal, and that deaths, on the average, are valued at $300,000. Obviously, there is much debate over the applicability of such a number, or any number, to human life. The derivation of this number is discussed by Moll et al. (1975).

Severe chronic human effects are also valued at $300,000, and recoverable at $30,000. Crop yield losses are valued at three cents per square meter (Bureau of the Census, 1974b).

A.4.7 Mathematical Formulation

The foregoing paragraphs have described the air pollutant component of the hazard ranking in generally qualitative terms. The actual hazard value for air pollutants is computed according to the formula given in Section A.3.2.1, with the concentration given by

$$C_{ijmnk} = c_{ijmnk} Q_{ijm}(3 \times 10^{-5})$$

where C is the concentration in $\mu g/m^3$, c_{ijmnk} is the concentration multiplier for the coordinates associated with group k of population type n from chemical i emitted from source j to medium m = air, in $\mu g/m^3$ per g/sec, Q_{ijm} is the emission rate of chemical i from source j to medium m = air, in kg/yr, and the constant converts kg/yr to g/sec.

A.5 WATER POLLUTANTS FROM MUNITIONS PLANTS

Only surface water, and in particular only rivers, are assumed to be directly polluted by munitions plant effluents.

A.5.1 Sources

The water pollutants listed in Tables A.5-1 and A-5.2 are thought to be discharged to rivers during the manufacture of explosives and primers and the loading and packing of shells. Relatively well-known discharge rates are shown in Table A.5-1. Additional estimates, based on

Table A.5-1

MAJOR WATER POLLUTANTS

Pollutant	Code	Estimated Waste (lb/mo)	Processing Rate (lb/mo)	Plant
Nitroglycerin	NG	2560	500,000	RAAP
Trinitrotoluene	TNT	1325	3,000,000	NAAP
		2650	6,000,000	VAAP
		3975	9,000,000	RAAP
		7950	18,000,000	JAAP
		3200	Loading only	HAAP
Trinitroresorcinol	TNR	450	3,500	LCAAP
Tetracene	TZ	110	800	LCAAP
Lead styphnate	PBS	2400	8,700	LCAAP
PETN	PET	60	1,000	LCAAP
White phosphorus	WPH	1500	400,000	PBA
RDX	RDX	5000	10,000,000	HAAP
HMX	HMX	380	210,000	HAAP

Source: Rosenblatt et al., 1973; SRI

Table A.5-2

ADDITIONAL WATER POLLUTANTS

Pollutant	Code	Estimated Waste (kg/yr)	Plant	Remarks
Nitroguanidine	NGU	1.7×10^3	RAAP	
Chromium (hexavalent)		330	All LAP	Data not processed
Glycerol-1,3-dinitrate	13D	1.2×10^4	RAAP	Hydrolysis of nitroglycerin
Glycerol-1,2-dinitrate	12D	1.4×10^3	RAAP	Hydrolysis of nitroglycerin
Glycerol-1-nitrate	1MG	9×10^3	RAAP	Hydrolysis of nitroglycerin
Glycerol-2-nitrate	2MG	180	RAAP	Hydrolysis of nitroglycerin
2,6-dinitrotoluene	26D	80	VAAP	Associated with TNT
		130	RAAP	
		260	JAAP	
		100	HAAP	
2,4-dinitrotoluene	24D	4.2×10^3	VAAP	Associated with TNT
		6.6×10^3	RAAP	
		1.3×10^4	JAAP	
		5.1×10^3	HAAP	
4-amino-2,6-dinitrotoluene	4AD	450	VAAP	Associated with TNT
		700	RAAP	
		1400	JAAP	
		560	HAAP	
2-amino-4,6-dinitrotoluene	2AD	450	VAAP	Associated with TNT
		700	RAAP	
		1400	JAAP	
		560	HAAP	
2-nitrodiphenylamine	NDP	100	RAAP	
Cyclohexanone	CHX	1.7×10^5	HAAP	Associated with RDX/HMX
Hexamine	HEX	5×10^3	HAAP	Associated with RDX/HMX
SEX	SEX	30	HAAP	Associated with RDX/HMX

Source: SRI

fragmentary data or on transformation rates from primary compounds to degradation products, are shown in Table A.5-2.

The rivers thought to be receiving the discharges are the South Fork of the Holston River for HAAP, the Illinois River for JAAP, the New River for RAAP, and the Tennessee River for VAAP. Primers are manufactured at LCAAP and are presumably discharged into the Little Blue River. Groundwater pollutants at RMA (see Section A.6) are believed to move into the South Platte River. Attempts should be made to pinpoint the exact locations of discharge pipes to define the relative locations of all populations downstream of the discharge points.

A.5.2 Transport

Transport is assumed to take place as a result of the pollutant flowing downstream from the discharge points. Concentrations are determined principally through dilution by average and low flows of the polluted stream and of its downstream confluences. Impoundments, although identified as the likely sites for fish populations, are largely ignored in the model. Travel times of pollutant to population centers are required for the transformation and transfer models.

A.5.2.1 River Receiving Waters

The river systems polluted by munitions plants should be traced using USGS maps (7-1/2 minute quadrangles as well as 1:250,000 scale). Important downstream confluences are identified, as are major impoundments (reservoirs, lakes). Population centers potentially drawing water from the rivers are identified; and to the extent possible, it is determined whether they use groundwater or tributary surface water.

Pollutants introduced into the receiving waters are assumed to be instantaneously diluted; furthermore, the discharges are assumed to be constant over the entire year.

A.5.2.2 Average and Low Flow Dilution

Transport is assumed to take place through mass movement with, and dilution by, the entire stream flow. Two different conditions are considered.

First, chronic effects in humans and fish are assumed to be related to the average concentration in water, and thus dilution by the average river flow over the year is one condition of interest.

At the other extreme, acute toxicity in fish is likely to be observed only when the concentration peaks during low flow conditions. Thus, some measure of the low flow is also used for dilution calculations. However, the definition of low flow is subject to considerable interpretation. Usually, a flow rate corresponding to the lowest flow over 7 days expected once in 10 years (the "7Q10") should be used if available. Other low-flow data, of several different sorts, can be used when the 7Q10 is not reported. If no other data are available, the low flow should be assumed to be about one-seventh of the average.

Data on flow rates may be obtained from the USGS and other sources (often telephone calls to state offices). Flow rates can be given in units of ℓ/yr or CFS, but no correction factor is supplied as yet for acre-feet/yr. Effluent rates are ordinarily expressed in kg/yr. The resultant concentrations are usually expressed in mg/ℓ.

A.5.2.3 Confluences

Confluences, where the polluted stream enters a larger river, or where tributaries enter the polluted river, cause additional dilution. Thus, the total average and low flows in each reach between confluences may be determined and used for populations exposed to water in that reach.

A.5.2.4 Impoundments

Most of the rivers under consideration are controlled through a series of dams. Additional "impoundments" occur as natural lakes. Such impoundments have several effects on pollution hazards, most of which are ignored in the present system.

First, the impoundments support large fish populations. Most of the fish populations identified in the system so far are associated with impoundments.

Second, reservoirs serve as buffers for downstream concentrations. Although some flow through reservoirs occurs without any real mixing, the downstream concentrations tend to be biased toward the average through the buffering of the reservoir. However, no provision for such averaging has been included in the system, and peak concentrations are assumed to be related to local low-flow conditions.

Third, reservoirs tend to increase the transit time of the pollutant. Although a given molecule could travel through a reservoir at the velocity of the input and output streams, the average molecule will remain in the reservoir much longer. Thus, there will be more chance for transformation or transfer. This phenomenon, too, has been ignored, making the peak concentration calculation conservative.

A.5.2.5 Pollutant Travel Times

Pollutant travel times to points downstream are important for calculating concentration decreases through transformation and transfer. These times are sometimes available directly, as for rivers under TVA control. For others, it is necessary to measure the downstream distance and estimate the river velocity. If the velocity is not known, it can sometimes be estimated from the flow rates and the river cross sections. However, the latter are typically difficult to determine. If no other information is available, velocities are assumed to be about 0.3 m/sec.

A.5.3 Transformation and Transfer

Transformation and transfer of chemicals are handled simultaneously in the models. Only an overall rate constant for the chemical's disappearance from the water is used as an input to the computer model. All component rates are estimated and combined by manual procedures described in Annex A.B.3.

A.5.3.1 Chemical Transformation

Estimates have been made for chemical transformation in surface water by hydrolysis, photolysis, oxidation, and biodegradation. Half-lives are estimated for each process and the corresponding rate constants are computed and summed to give a total rate constant for chemical transformation. Hydrolysis, photolysis, and biodegradation seem to be more important than oxidation for most of the chemicals studied, but some chemicals oxidize. Very little information is available on biodegradation, and the correct half-lives for chemicals in flowing water are very uncertain. Total estimated half-lives range from a few hours to several years or even decades. If a process is known to occur, but the rate is unknown, a default value of 1 year for the half-life is usually used.

A.5.3.1 Physical Transfers

Estimates have also been made for the half-lives and rate constants for transfers to air by evaporation and to sediments by precipitation and adsorption. These estimates are based on vapor pressure, molecular weight, and water solubility in the case of evaporation (MacKay and Wolkolf, 1973), and principally on solubility in the case of sediment transfers. These predictions span at least as large a range as the chemical transformation, and similar default assumptions are used.

After the transformation and transfer rate constants have been determined, the two are added together to produce an overall rate constant for disappearance of the chemical. This overall rate constant is used with the time of travel to the populations-at-risk in an exponential decay function that modifies the concentrations calculated by dilution alone.

A.5.4 Exposure

Exposure from water pollutants are calculated differently for human and fish populations. For human populations, such exposures can be concentration dependent or dose dependent.

A.5.4.1 Human Exposures

Human exposures are calculated beginning with the average flow-rate concentrations, as computed in the local reach of the river (source water). It is assumed that the source water is passed through some sort of water treatment plant before being delivered as drinking water (finished water). The treatment efficacy is defined as the ratio of the pollutant concentration in the finished water to that in the source water.* This ratio will vary from chemical to chemical and for a given chemical from treatment plant to treatment plant.

The treatment efficacies are generally not known with any certainty. In particular, no information has been developed to model the variation in the ratios with different treatment combinations. Consequently, default values for several of the chemicals have been developed and are shown in Table A.5-3.

Table A.5-3

WATER TREATMENT EFFICACIES

Treatment Efficacy*	Chemicals Included†
1.0	TNT, TNR, PET, 24D, 26D, CHX
0.9	CHL
0.8	2AD, 4AD
0.5	NG, NGU, RDX, HMX, 13D, 12D, SEX, TDG, LWO, MPA, IMP, DMP, DPD, TZ
0.3	PBS, 1MG, 2MG, NDP, HEX,
0.01	WPH

*Ratio of concentration in finished water to that in source water. (1.0 = 0% removal, 0.5 = 50% removal.)

†Identification code--see Tables A.5-1 and A.5-2.

Source: SRI.

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*Note: High values of this ratio (near unity) imply little treatment efficacy. The definition is in some ways an inverse one.

To determine concentration-dependent effects in humans, the concentration of pollutant in the finished water is computed by multiplying the concentration in the source by the treatment efficacy. To estimate dose-dependent effects, the annual dose is computed by multiplying by the drinking rate, 500 ℓ/yr. This drinking rate probably overstates the dose, because it includes milk, beer, soft drinks, and so on, that might not be made from the source water. However, it does not include water in food or water of metabolism.

A.5.4.2 Fish Exposures

Fish exposures for acute toxicity and chronic toxicity are equal to the concentrations calculated from the low-flow and average river dilution factors, respectively, for the reach of the river in which the fish population is located.

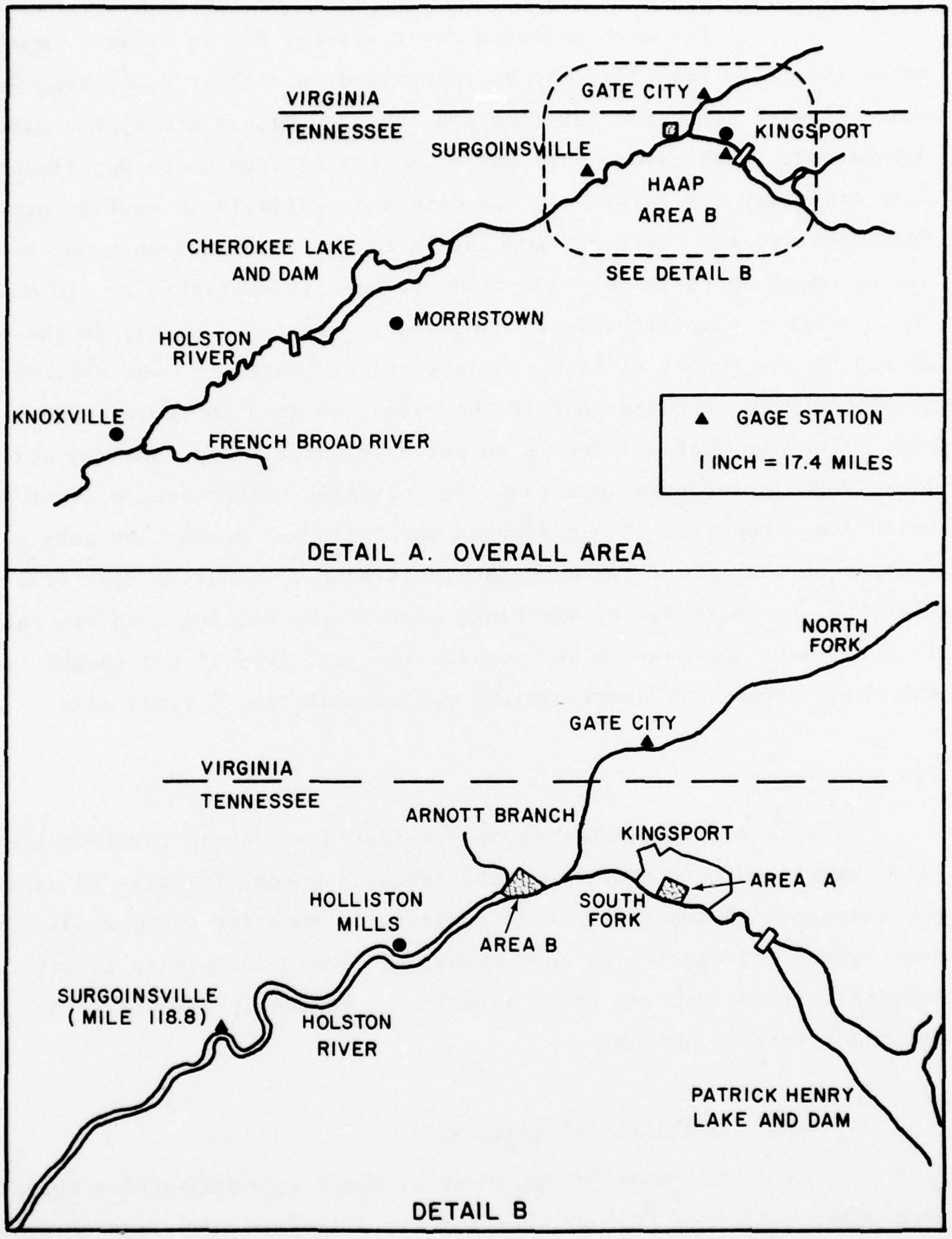
A.5.5 Populations-at-Risk

As explained above, the only populations considered to be at risk from water pollutants are humans and fish.

A.5.5.1 Humans

The human populations-at-risk are those taking their drinking water from the polluted streams. Those on wells or other surface sources are not at risk.

The communities taking water from the polluted streams should be identified through Army reports (Figure A.5-1), USGS maps, and contacts with state and local governments. In doubtful cases, it should be assumed that the community in question does take river water. The populations are determined from census information, maps, or commercial atlases. In cases for which river water is taken only part of the year, the fraction can be applied to the population to obtain an equivalent population.



SOURCE: Rosenblatt, et al. 1973.

FIGURE A.5-1 MAP OF HOLSTON ARMY AMMUNITION PLANT AREA

A.5.5.2 Fish

For each polluted river system, one to several impoundments likely to have fish may be identified, and their downstream distance, travel time, and low flow and average ingress and egress rates determined. Fish census data may be solicited from state departments of fish and game, but relatively few data are available in useful form. Consequently, the "natural" population may be estimated on a per-acre basis, using approximately 200 fish per acre (0.05 fish/m^2). In doing this, several simplifications should be recognized. First, in the estimation of the number of fish, the equivalent number of "one-dollar" fish should be used, because that is the value assigned in Table A.3-4. Second, it may be that a river is so polluted, usually by non-Army activities, that is supports less than the "natural" number even without Army pollution. However, if one assumes the "natural" number, he gets a prediction of the effects of Army chemicals alone. Finally, most fish populations are augmented by stocking; most of the stocked fish are caught in a few days and many do not survive the year even if not caught, so they have relatively short periods for accumulating a toxic dose.

A.5.6 Effects

The water pollution effects considered are human carcinogenicity, other severe chronic and recoverable chronic human effects, and acute and chronic fish toxicity. Crop toxicity is thus far assumed unimportant because irrigation in most areas near munitions plants is rare. Effects in livestock and other animals are currently assumed to be less important than in humans.

A.5.6.1 Human Carcinogenicity

The model's treatment of human carcinogenicity resulting from water pollution follows that for air pollution (see Section A.4.5.1) except that probabilities and potencies by the oral route are used. Total annual dose is used as the determinant of exposure.

A.5.6.2 Other Chronic Human Effects

Other chronic human effects of ingested pollutants (oral exposures) may be estimated on a chemical-by-chemical basis. Only a few potential effects have been identified (see Table A.5-4). For the remaining chemicals, default values are used as for air pollutants.

Table A.5-4

OTHER CHRONIC HUMAN EFFECTS FROM
WATER POLLUTANTS

Effect	Chemical	S (fraction per mg/kg)
Mortality	Nitroglycerin	2.0
	White phosphorus	0.25
Cardiovascular effects	PETN	0.25

Source: SRI

A.5.6.3 Acute and Chronic Fish Toxicity

Acute fish toxicity is assumed to be dependent on peak concentrations, as calculated from low-flow dilution. Most dose-response relationships are based on LC_{50}, the lethal concentration for a 50% fish kill. Measured dose-response relationships typically have a substantial nonzero threshold followed by a steep sloping function to saturation (100% fatalities), that is, toxic effects occur over a narrow range of concentrations. However, the curves have been reinterpreted to be of zero threshold by extrapolating linearly from the 5% response point to the origin (see Annex A.B.5.2). No toxicity was assumed for chemicals for which no data were found.

Chronic toxicity data are not generally available, but slopes can be given default values, often about 20 times acute values, if the latter are known.

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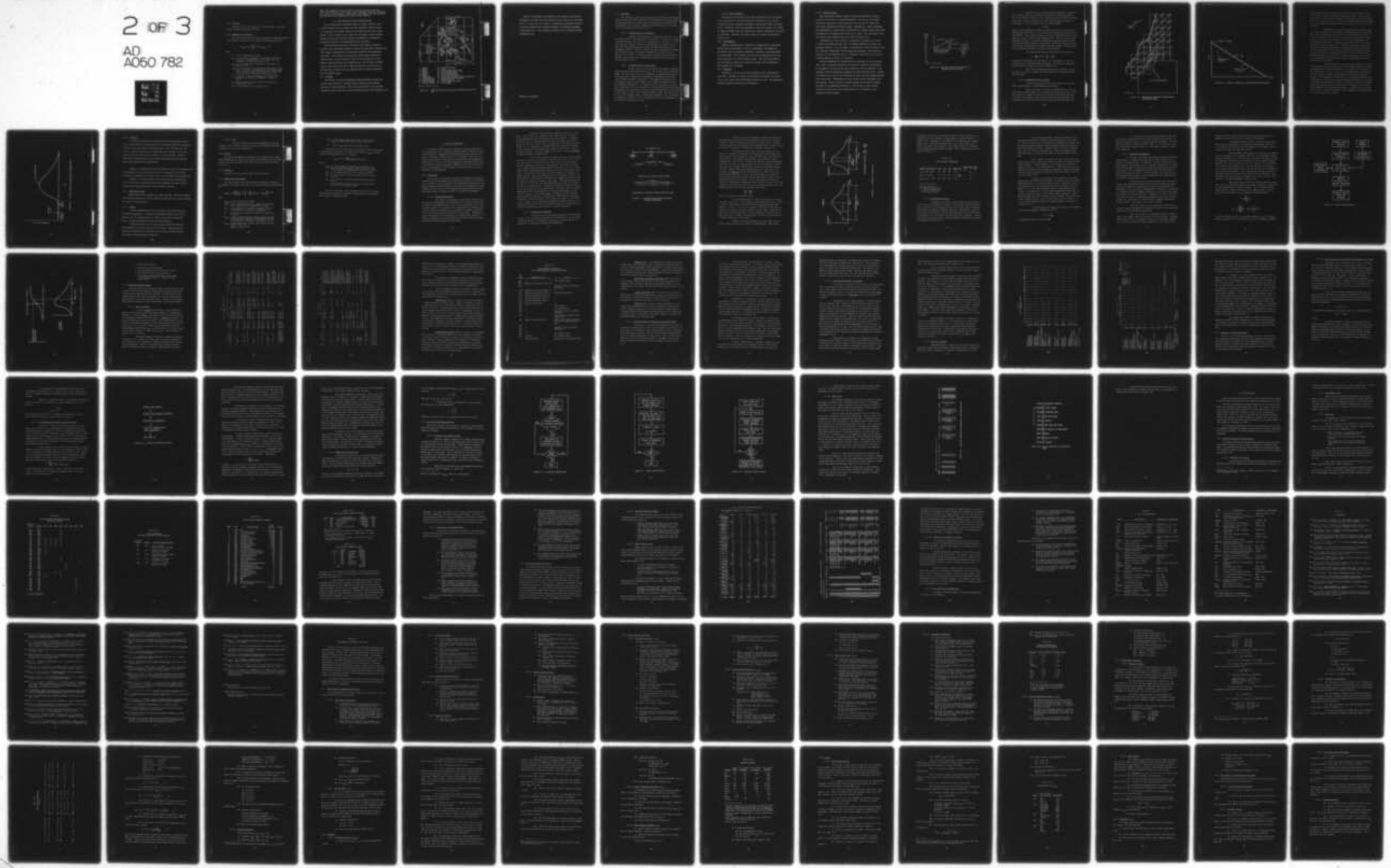


A.5.7 Valuation

The human effects are valued as for air pollutants. All cases of fish toxicity are valued at \$1/fish.

A.5.8 Mathematical Formulation

The actual hazard value for water pollutants is computed according to the formula of Section A.3.2.1, with the concentration given by

$$C_{ijmnk} = R_{in} \frac{Q_{ijm}}{f_{jnk}} \exp(\lambda_{im} t_{jnk}) \times 10^6$$

where

C	is the concentration in mg/ℓ
R_{in}	is the treatment efficacy for pollutant i and population type n, dimensionless: if n = FSH, $R_{in} = 1$; otherwise, it is given by Table A.5-3
Q_{ijm}	is the effluent rate of chemical i from source j to medium m = water
f_{jnk}	is the flow rate of the river reach downstream of location i for group k of population type n, using average rates for human effects and chronic fish toxicity and low-flow rates for acute fish toxicity, in ℓ/yr
λ_{im}	is the sum of the transformation and transfer rate constants for chemical i in medium m = water, in $(\text{yr})^{-1}$
t_{jnk}	is the transit time from location i to group k of population n, in yr
10^6	is the conversion factor from kg to mg.

NOTE: The submitted version of Chapter A.6 cited specific pollutants which are the subject of litigation. Certain sections, taken out of context, could affect this litigation. Accordingly, this chapter has been rewritten. The page order of the submitted version has been retained.

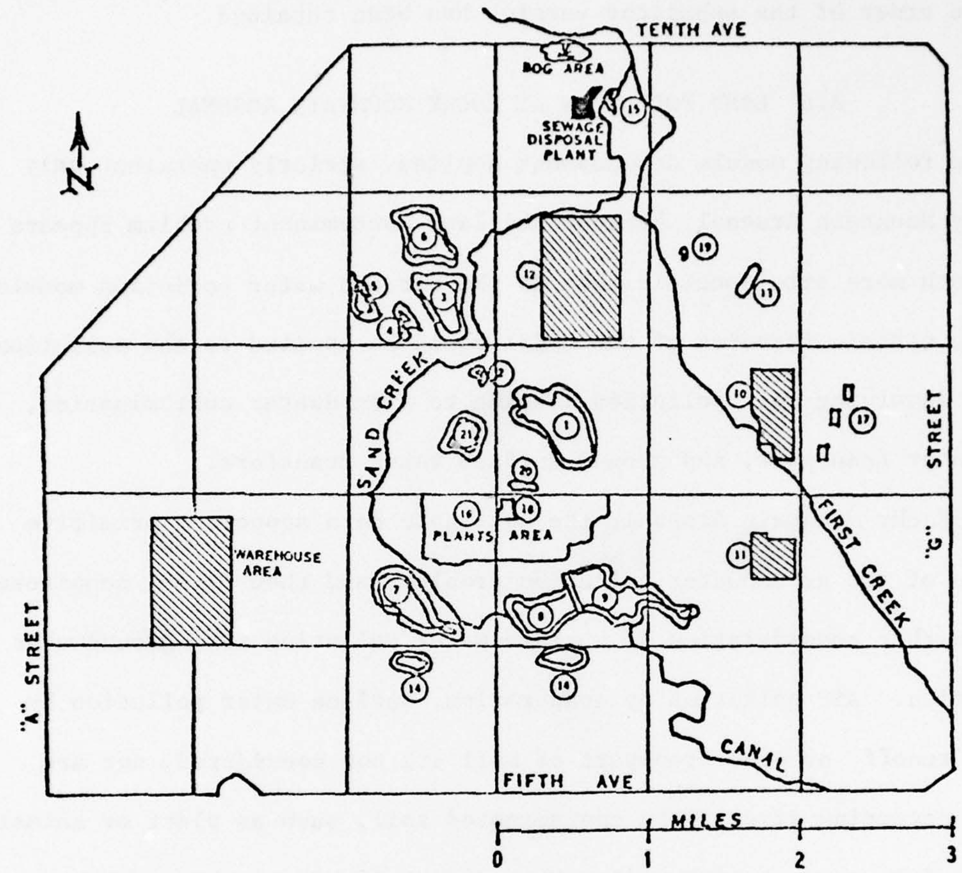
A.6 LAND POLLUTION AT ROCKY MOUNTAIN ARSENAL

The following module development applies, strictly speaking, only to Rocky Mountain Arsenal, because the land contaminant problem appears to be much more site-specific than do the air and water pollution models. However, certain features of the model could be applied to any pollution problem involving soil pollution leading to groundwater contamination, groundwater transport, and ground-surface water transfers.

At Rocky Mountain Arsenal, the available data support a primitive analysis of the groundwater pollution problem, and theoretical considerations allow further consideration of surface water pollution from groundwater percolation. Air pollution by evaporation, surface water pollution by surface runoff, or dust transport of soil are not considered, nor are effects occurring directly in contaminated soil, such as plant or animal toxicity from contact with soil. This discrimination is based more on available data and models than on assurance that the effects considered are the dominant hazard.

A.6.1 Sources

The sources of pollution include past Army activities and past and current lesee activities. Although disposal activities have spanned many areas in RMA (Rosenblatt, 1975), the principal sources of pollution considered in this study were the waste disposal Basins A and F (Figure A.6-1).



1. BASIN A
2. BASIN B
3. BASIN C
4. BASIN D
5. BASIN E
6. BASIN F
7. LADORA LAKE
8. LOWER DERBY LAKE
9. UPPER DERBY LAKE
10. CHEMICAL STORAGE
11. CHEMICAL STORAGE
12. GB DEMILITARIZATION
13. LANDFILL
14. DIELDRIN-CONTAMINATED SLOUGHS
15. BURIED ANTICROP AGENT
16. SHELL CHEMICAL COMPANY
17. BURNING PITS (INACTIVE)
18. MUSTARD DEMILITARIZATION (OVER OLD LIME PITS)
19. EXPLORATION FOR BURIED CHEMICAL CONTAINERS (EMPTY)
20. SETTLING PONDS (LIME PITS)
21. CAUSTIC BASIN

SOURCE: Rosenblatt, et al. 1975.

FIGURE A.6-1 CONTAMINATED AND POTENTIALLY-CONTAMINATED AREAS AT RMA

Almost no information is accessible on the amounts of contaminants discharged to the basins or other locations, and it may well be that none exists. In many ways, it is better to establish an equivalent reservoir by working backwards from empirical treatments of observed groundwater concentration data. This estimation technique will be further discussed immediately below.

[Table A.6-1 Deleted]

A.6.2 Transfers

The transfers of pollutants assumed to be occurring at RMA include transfer from soil (basin reservoirs) to groundwater by leaching, transfer from groundwater to surface water by percolation, adsorption from groundwater to soil surfaces, evaporation from soil surface, and evaporation and adsorption from surface water.

A.6.2.1 Introduction into Groundwater

Transfer into groundwater is assumed to take place at a rate proportional to the remaining soil inventory. It is further assumed that this injection takes place at a specific point. Finally, it is assumed that the original reservoir was established at a unique point in time, and has been decreasing ever since through evaporation and the groundwater transfer. Since in reality the soil contamination took place over a period of time, the assumed formation time is chosen near the middle of this period. In practice, when concentration values have been measured, the transfer rate is empirically estimated and the reservoir size is computed from it.

A.6.2.2 Introduction into Surface Water

At RMA, the water table intersects the ground topography along the banks of the South Platte River, and to some extent along First Creek. The total flow rate per unit length of the ground-surface water intersection can be computed by estimating the groundwater flow velocities, aquifer thickness, and porosity. The change in total flow rate of the South Platte per unit length in the region of interest can also be estimated independently. A comparison of these quantities indicates that essentially all of the groundwater is carried off by the South Platte. Consequently, all the pollutant load entering the South Platte is diluted by the flow rate of the river, whether average or high. The source term for the river transport model, as described in Section A.5.2, is given by the integral of pollutant flows in groundwater over the intersection of the pollutant field with the river.

A.6.2.3 Other Transfers

Evaporation rates from soil (the basin reservoirs) to air are assumed to be essentially the same as they would be from water to air, and are estimated from vapor pressure, solubility, and molecular weight (see Annex A.B.3). Adsorption rates from groundwater to soil are assumed to be similar to sediment transfer rates for surface water, and are estimated on the basis of solubility. Transfers from surface water are treated as described in Section A.5.3.

A.6.3 Tranformation

Chemical transformation is assumed to be taking place by hydrolysis, oxidation and biodegradation in soil, by hydrolysis, and oxidation in groundwater, and by hydrolysis, photolysis, oxidation, and biodegradation in surface water. Rate constants are estimated as described for air and water pollutants, with similar default values. The total rate constant for each medium is computed by summing the transfer and transformation rate constants for the medium.

A.6.4 Transport

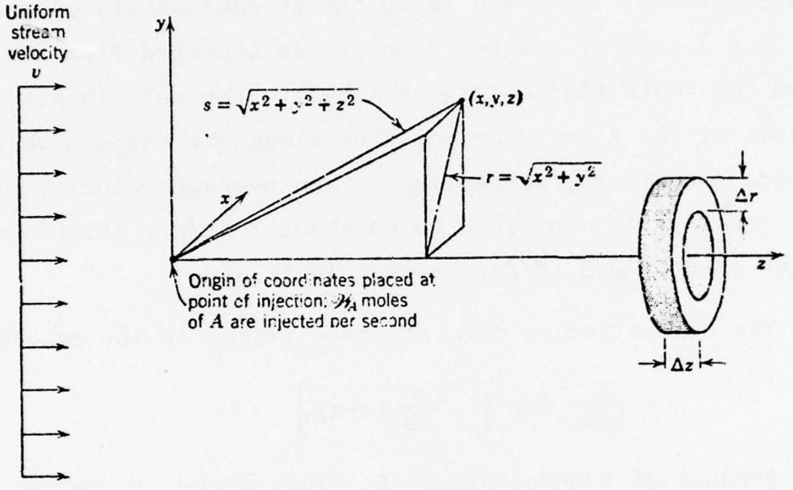
Transport in air or in soil (dust transport) is not considered in this model. Transport in surface water follows the treatment of Section A.5.2, with a source term ad described in Section A.6.2.2. The significant transport problem at RMA occurs in groundwater.

A.6.4.1 Diffusion Model

Most groundwater transport models are extremely complicated, usually occurring in the form of a detailed simulation. Not only do these models suffer from limitations on input data, but they are also too complex for this hazard estimating and ranking system. Consequently, a simple diffusion model applicable to a point source of pollution in a uniform laminar flow field is adapted for the present system (Bird et al., 1962). The definitions of the flow velocity and coordinate system are shown in Figure A.6-2.

Concentrations of the pollutant in groundwater are given by the model in terms of the pollutant input rate the average groundwater velocity, the downstream distance z, and the range s, as discussed in detail in Section A.6.9. The formulation incorporates two key adjustable parameters, the diffusivity constant D and the injection rate Q. Although in theory the latter could be directly measured, in fact it is inferred.

Certain assumptions and modifications were necessary to use this model. First, they y (vertical) coordinate was suppressed, and only concentrations in the plane of the source point were considered. This is equivalent to the assumption that all groundwater withdrawls are taken from this plane. Second, the velocity to be used in the formulation is taken to be the average velocity in the flow field. Determination of this velocity will be discussed in the next section. Third, the path of maximum gradient in the bedrock altitude was taken as the downstream direction, z, and contours of equal bedrock altitude was taken as the cross-stream direction, x, regardless of the curvature of these contours.



SOURCE: Bird, et al. 1962.

FIGURE A.6-2 DIFFUSION FROM A POINT SOURCE IN A CONSTANT-VELOCITY STREAM

The first step is to calculate the groundwater parameters for each well sampled. The basic data are obtained from hydrogeologic maps of the RMA area (Konikow, 1975), showing contours of bedrock altitude, water table altitude, transmissivity, and saturated aquifer thickness. Velocities, v, can be computed in m/sec from the formula

$$v = g\ TR/d$$

where g is the gradient in bedrock altitude (m/m), d is the thickness of the saturated water table, in m, and TR is the transmissivity of the aquifer (m^2/sec). Then a path of maximum velocity is sketched from the source point out toward the South Platte (Figure A.6-3). The well locations are described in terms of the z and x coordinates along the maximum velocity path and the bedrock contours, respectively. An average velocity path to the vicinity of these wells was found to be about 2 ft/day (0.007 cm/sec), but the variation spanned 0.5 ft/day to over 10 ft/day.

The concentration data are then fitted to the equation

$$C = \frac{Q}{4\pi Ds} \exp\left[-\frac{v}{2D}(s-z)\right]$$

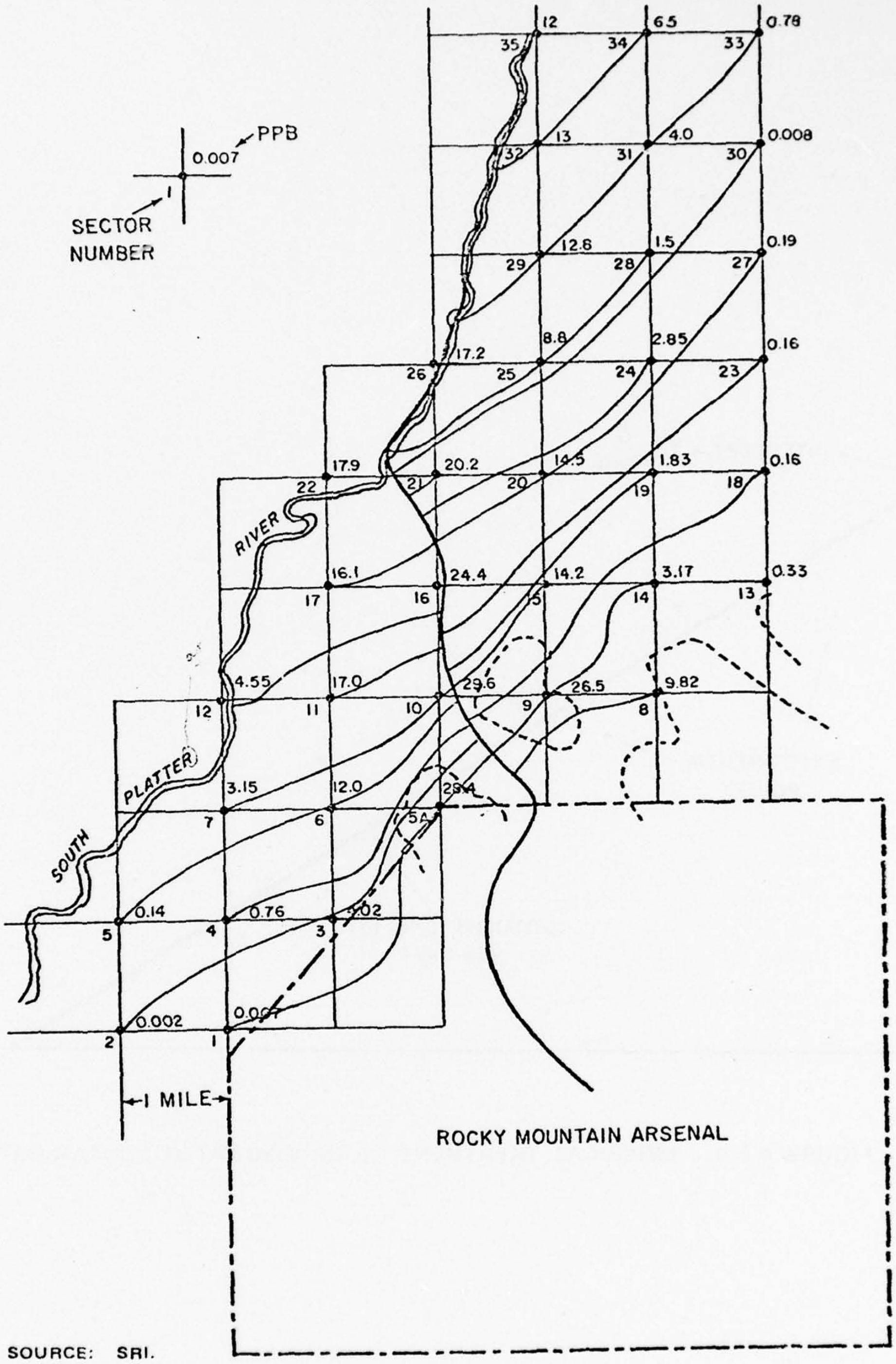
by plotting the product of concentration, C, times range, s, versus the quantity (s-z) on semilogarithmic graph paper. The intercept and slope give estimates of Q and D, as shown in Figure A.6-4.

Once these two parameters Q and D are estimated, the same equation can be used to compute the concentration at any other point in the flow field.

A.6.4.3 Difficulties with the Model

Several difficulties are associated with the use of the simple diffusion model for RMA groundwater pollution.

First, the model is a static or steady-state one, and assumes that a constant injection of pollutant has been going on for a long time, so that no changes in concentration with time are being observed. In reality, the injection rates are decreasing with time (assuming a decreasing source reservoir and constant transfer rate coefficients), and



SOURCE: SRI.

FIGURE A.6-3 **Hypothetical Pollutant Concentrations by Diffusion Model**

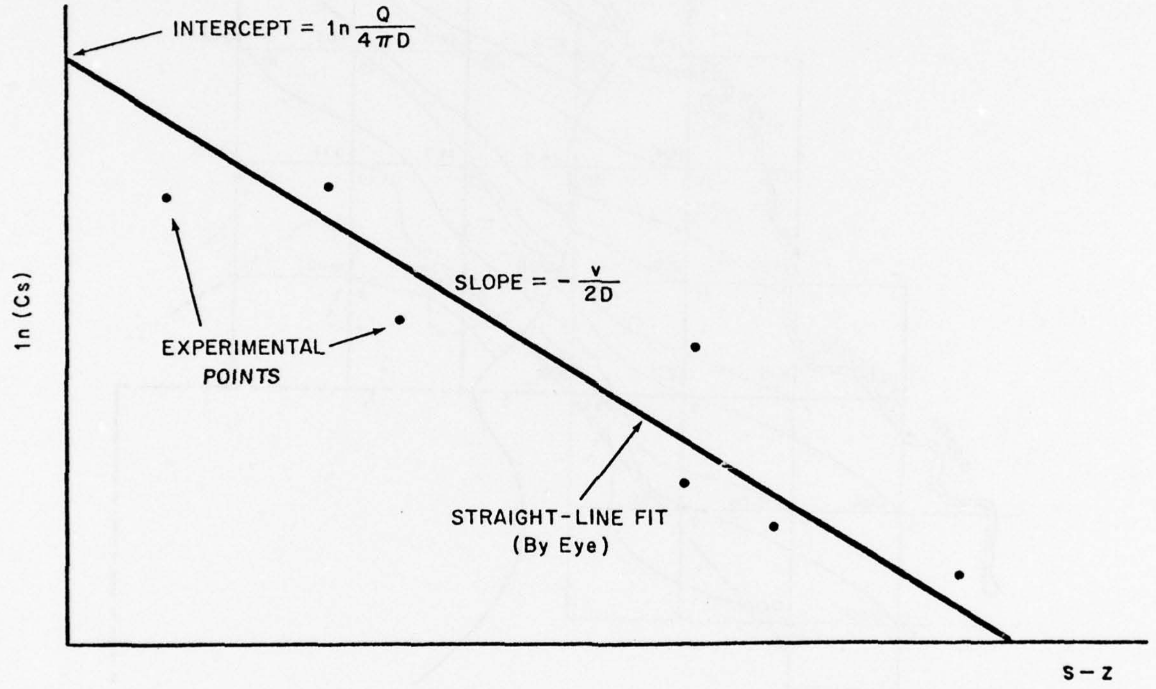


FIGURE A.6-4 EMPIRICAL TREATMENT OF GROUNDWATER CONTAMINATION furthermore, the injection started relatively recently, compared with travel times in the very slow-moving groundwater field. The most prominent effect is that the model predicts some nonzero concentration everywhere in the field, whereas in reality no concentrations are found beyond the distance that the goundwater could travel since the time of first injection.

Consequently, a method for predicting the variation with time of the concentration at any point is needed and should be developed. The critical variables are the time of first injection and the travel time to the point of calculation. The latter may be estimated to first order by s/v (range over velocity), but in reality the phenomenon is somewhat more complicated. A typical concentration pulse for a point in the field is shown in Figure A.6-5. Note the lag period, and the fact that the concentration peaks before declining. Presumably, the hazard due to a particular well is greatest during the year in which the peak concentration occurs. However, these peaks occur at different times at different locations, and the year of aggregate peak hazard for all the wells depends on the detailed distribution of populations-at-risk and cannot be easily predicted.

A second difficulty is that the model applies to a problem controlled only by diffusion, with no provision for pollutant removal by transformation and transfer; that is, the pollutant is considered to be "conservative." This in itself is not a problem, because the phenomena of transport, transfer, and transformation should be separable. However, the coefficient of diffusivity, D, is determined empirically by a graphical fit to data from a real concentration field that is affected by transfer and transformation as well as diffusion. Thus, the observed diffusion coefficient must be separated into a component for diffusion and a component for nonconservative effects. The correct way to do this would require a much more significant understanding of all the phenomena that can be justified at present.

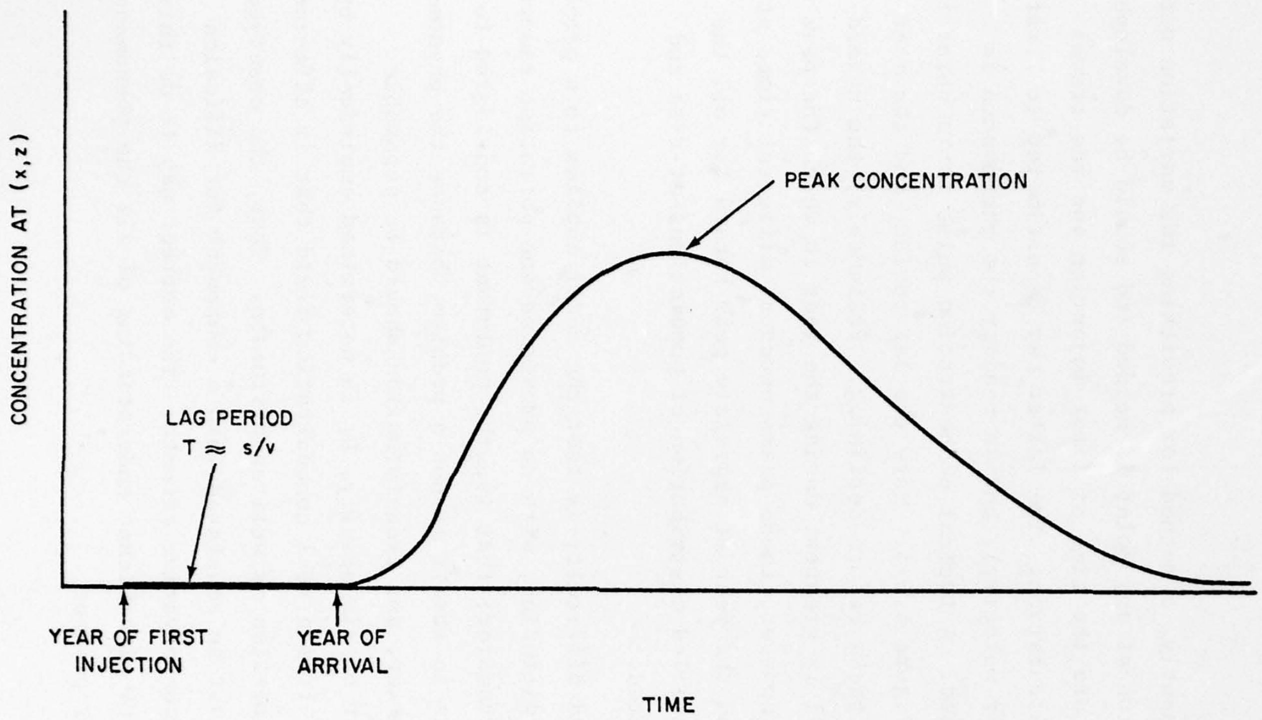


FIGURE A.6-5 A TYPICAL PULSE OF GROUNDWATER CONTAMINATION

A.6.5. Exposure

At present, groundwater concentrations and the corresponding surface water concentrations in the South Platte are calculated through the unadjusted transport model operating on 1974 measured data. Since the model fits the data, it should extrapolate well to unmeasured well locations, even if the time variation and nonconservative factors are not well known. Only the limitation of concentrations to zero beyond the penetration radius for the pulse should modify these extrapolations.

Exposures to human populations are determined either by the concentration in groundwater or by the dose predicted from the drinking rate. No water treatment of groundwater is assumed, that is, the treatment efficacy equals one.

Exposures to fish populations are given by the peak concentrations in the South Platte as determined by low-flow conditions for acute toxicity and by average concentrations and flows for chronic toxicity.

A.6.6 Populations-at-Risk

Populations-at-risk considered are humans and fish. Livestock, wildlife, and wild plant populations should be added when sufficient data become available. Crop losses are also possible.

A.6.6.1 Humans

The human populations-at-risk are assumed to be those that drink contaminated groundwater. Drinking of contaminated surface water is also possible, but the concentrations are likely to be an order of magnitude lower, and these populations have not yet been estimated.

Population centers in the vicinity (about 10 miles) of RMA have been identified in the area north of the two basins. Their populations have been determined from a commercial atlas and from estimates based on the number of buildings shown on USGS maps.

A.6.6.2 Fish

The South Platte has no major impoundments in the near vicinity of RMA. However, reaches of the river near Brighton and near Greeley were taken to be representative.

A.6.7 Effects

The effects considered are the same as for surface water, namely, human carcinogenicity, other severe chronic and recoverable chronic human effects, and acute and chronic fish toxicity, and are discussed in Section A.5.6.

A.6.8 Valuation

Valuation is as for surface water (see Section A.5.7).

A.6.9 Mathematical Formulation

The actual hazard value for groundwater pollutants is computed according to the formula of Section A.3.3.1, with the concentration given by

$$C_{ijmnk} = \frac{Q_{ijm}}{4\pi D_{ij} S_{ijnk}} \exp\left[- \frac{V_j}{2D_{ij}} \left(S_{ijnk} - Z_{ijnk} \right) \right] \times 10^6$$

where

C_{ijmnk} is the concentration in mg/ℓ

Q_{ijm} is the estimated injection of chemical i from location j into medium m = groundwater, in g/sec

D_{ij} is the observed or calculated diffusion constant for chemical i at location j, in cm^2/sec

V_j is the average velocity of the field at location j, in cm/sec

Z_{ijnk} is the distance along the maximum velocity gradient to the location of group k of population n from the discharge spot of chemical i at location j, in cm

S_{ijnk} is the "slant range" between those points, given by $\sqrt{X^2_{ijnk} + Z^2_{ijnk}}$, where

X_{ijnk} is the distance along the contour of constant bedrock altitude between these points, also in cm, and

10^6 is the conversion factor from g/cm^3 to mg/ℓ

Concentrations in surface water are predicted by the dilution equations discussed in Section A.5, based on the input rate Q_{ijm}, in kg/yr, derived as described in A.6.2.2. Formally,

$$Q_{ijm} = 3.2 \times 10^7 \sum_k C_{ijmnk} TR_{jk}\ g_{jk}\ L_{jk}\ P_j$$

where

C_{ijmnk} is the groundwater concentration of chemical i at some point along the river, defined by indexes k and n, for medium m = groundwater at location j, in mg/ℓ

TR_{jk} is the transmissivity in that vicinity, in m^2/sec

g_{jk} is the gradient in bedrock altitude in that vicinity in m/m

L_{jk} is a length of river bank represented by that point, in km

P_j is the porosity (fractional) in the vicinity, taken to be 0.4 for location j = RMA.

The sum is carried out over contiguous stretches of river bank associated with significant groundwater concentration levels (roughly from Irondale to Brighton at RMA).

A.7 ALLOCATION METHODOLOGY

Section A.2, especially A.2.4, explains in general terms that an index of preference for a candidate research study is expressed in terms of the difference in aggregate hazard-uncertainty before and after the study is conducted, divided by the cost of the study. This section explains in more detail (1) the process of estimating and propagating uncertainties in the values for input variables to the hazard calculations, (2) the types of studies conducted by EPRD and their cost and effectiveness, (3) calculation of the difference in hazard uncertainty, and (4) operation of the methodology.

A.7.1 Uncertainty

The concepts of uncertainty in values of measured and calculated variables that are developed here are difficult to defend in any rigorous sense. However, they are considered to be reasonable descriptions of the desired research allocation problem, and should give significantly better insights into the most effective research areas than do currently available methods based on informed opinion and qualitative assessments.

A.7.1.1 Bayesian Uncertainty

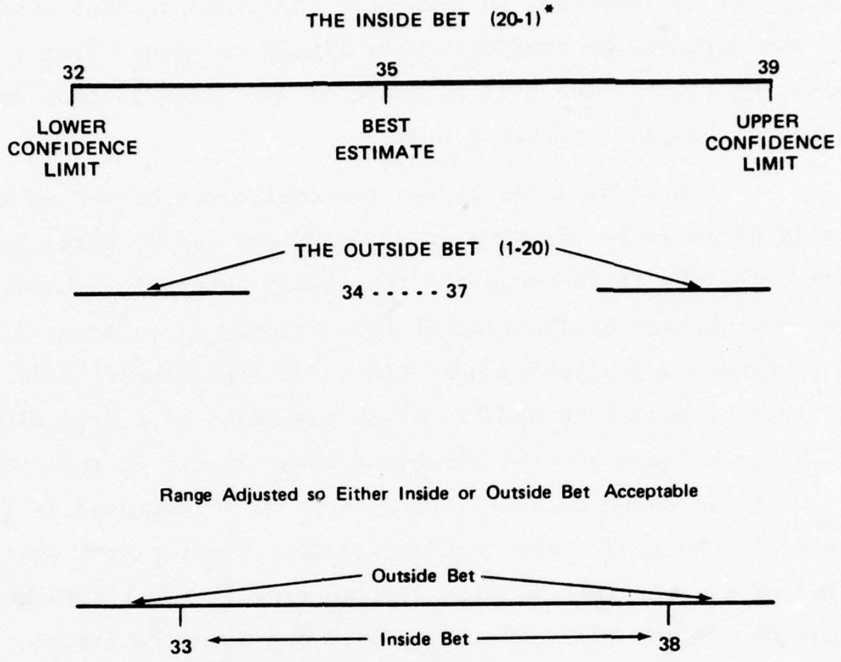
The underlying assumption of uncertainty estimation for the allocation methodology is that uncertainty in variable values should be viewed in the Bayesian sense. That is, the uncertainty is not a statistical property of the variable or its measurement, but instead represents the subjective confidence of an observer or observers (operators of the system) that the value lies within a given range. The Bayesian view of uncertainty is not accepted by all statisticians; however, it is the most convenient view for analyzing choices under conditions of great uncertainty and few experimental observations.

Suppose an analyst wants to estimate the value of a variable x. His first job is to select a value that is his best estimate ($\hat{x}$) considering the state of knowledge about that variable. In doing so, he may have access to measured data, may make an estimate on scientific grounds, or may use a default value, as explained in Sections A.3-A.6 and Annex A.B. It is important to recognize that this current best estimate is also the estimate he considers most likely to result from a study to determine the value. The best estimate of the value is thus not <u>expected</u> to change, although it probably will.

Next he investigates the confidence he has in this estimate. How easily could it be 50% greater? Two-thirds less? What, in fact, are the limits that he feels bound all the likely values for the variable? The most commonplace explanation of this process is in terms of placing a bet. Suppose the analyst's best estimate of the value of x is 35. Then suppose that he were betting 20 to 1 that the value of x fell within a given range. He might then set the upper and lower limits of this range as 32 and 39. This is known as the "inside bet," as illustrated in Figure A.7-1. Alternatively, he could take the "outside bet," wagering 1 against 20 that the value of x would fall outside a given range. The limits he would now set might be <34 and >37. When the upper and lower limits of the range are set so that the analyst is indifferent to whether he takes the inside bet or the outside bet, he has adjusted the "confidence limits" to enclose approximately 95% of the probability he subjectively assigns to values for the variable. In the above example, he might adjust the lower and upper limits of the range to 33 and 38 and be indifferent as to whether he bet 20 to 1 that the value of x fell within this range, or 1 to 20 that it fell outside. These subjectively determined confidence limits are assumed to be equivalent to the 95% confidence limits for a subjective statistical distribution of the outcomes of a perfect experiment.

A.7.1.2 <u>Statistical Terminology</u>

In spite of the fact that Bayesian subjective uncertainty is used in the allocation methodology, it is convenient to use the terminology and concepts of conventional statistics to describe many of the properties of uncertainty estimation and propagation.



* Subjective estimate of the probability of obtaining a value within the range.

FIGURE A.7-1 ESTABLISHING CONFIDENCE LIMITS FOR BAYESIAN UNCERTAINTY

First of all, it is convenient to think of a probability distribution that gives the relative subjective probabilities that the outcome of a perfect experiment would fall at various values. Because of prior exposure to such concepts, most scientists tend to think in terms of normal or log-normal distributions,as sketched in Figure A.7-2.

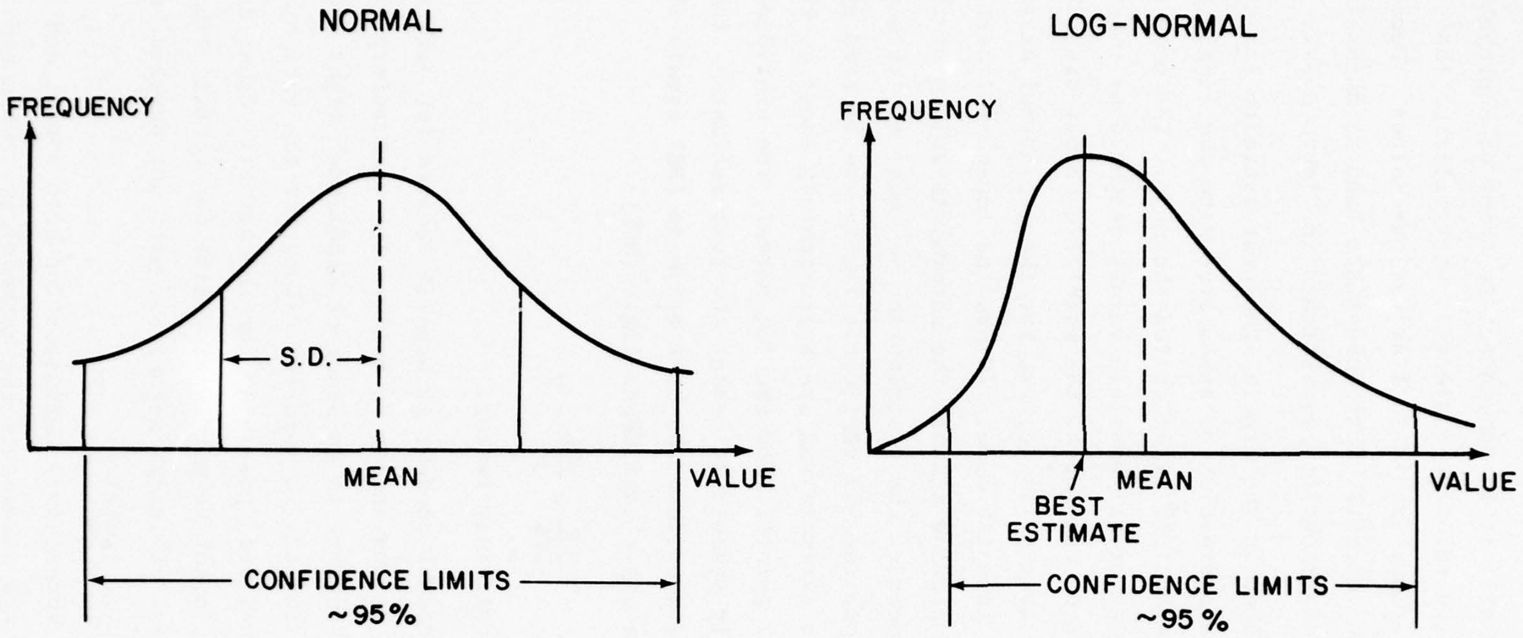
As indicated in the figure, the best estimate for the value of a variable would ordinarily be associated with the single most likely value of the distribution, often called the mode. The mean of the distribution is the average of all possible values weighted by their probabilities of occurrence. As shown, the mean of a normal distribution is equal to its mode, or best estimate, but for the log-normal distribution, the mean is higher than the mode. (Since the log-normal distribution looks "normal" when plotted against the natural logarithm of the variable, the geometric mean of the distribution is equal to the mode.) In the normal distribution, the 95% confidence limits are located symmetrically about the best estimate and are approximately equal to the two standard deviation (S.D.) points. For the log-normal, the confidence limits are logarithmically symmetrical about the best estimate: the lower confidence limit (LCL) divided into the best estimate (BE) equals the best estimate divided into the upper confidence limit (UCL):

$$\frac{\mathrm{BE}}{\mathrm{LCL}} = \frac{\mathrm{UCL}}{\mathrm{BE}} = \mathrm{U}$$

where U is called the uncertainty factor.

The log-normal concept is usually favored for very uncertain data because (1) it is convenient to think about uncertainty in terms of orders of magnitude--"correct to an order of magnitude" might mean UCL/LCL $\approx$ 10 or U $\approx$ 3.2, and (2) no negative values for the variable are possible--in contrast, they are "possible" for the normal. Other distribution, such as the beta, might be more appropriate for certain kinds of data, such as the treatment efficacy factor, but were not pursued because of their unfamiliarity to most users.

However, uncertainty estimates for both normal and log-normal conceptual models are allowed by the methodology. When coding



$$\text{UNCERTAINTY FACTOR} = \frac{\text{BE}}{\text{LCL}} = \frac{\text{UCL}}{\text{BE}}$$

FIGURE A.7-2 "STATISTICAL" TERMINOLOGY

uncertainty, the operator is allowed to specify either additively (+) or multiplicatively (*) symmetrical uncertainties. (Review column 49 in Figure A.3-4). Moreover, he can specify for the additive case ("normal" model) either a percentage uncertainty (% = p) or an absolute uncertainty (b = blank) (see column 55). The column 55 code for a multiplicative uncertainty should always be blank. These alternatives are illustrated in Table A.7-1.

Table A.7-1

WAYS OF CODING UNCERTAINTY

Example of Thinking	LCL	BE	UCL	Symbolism*	Uncertainty Code 49		55
$f_{jnk} = 500 \pm 150$	350	500	650	$A \pm B$	+	150	
$R_{in} = 0.5 \pm 20\%$	0.4	0.5	0.6	$A \pm A \frac{P}{100}$	+	20	P
$S_{im\ell} = 10^{-6} - 10^{-4}$	10^{-6}	10^{-5}	10^{-4}	$A \overset{\times}{\div} U$	*	10	

---

*A = Best estimate.
B = Absolute uncertainty.
P = Percent uncertainty.
U = Uncertainty factor.

A.7.1.3 Estimating Uncertainty

Although most scientists freely admit that their certainty in the value of a variable is incomplete, they are often extremely reluctant to quantify that uncertainty except in the classic sense of repeated observations and standard statistical analysis. Unfortunately, such luxuries cannot be afforded in a system that merely assists in the selection of experiments that would supply such firm statistical estimates. Instead, the system relies on subjective, rapidly generated estimates of uncertainty as described in Section A.7.1.1.

It will be uncomfortable for those unaccustomed to the allocation methodology to generate uncertainty estimates, and rightly so. There is a great deal of uncertainty in uncertainty estimation, and most people's first estimates of upper and lower confidence limits are not nearly conservative enough. However, there is a need for sticking one's neck out, and there is probably less risk of the analyst being wrong than there is if someone less expert is forced to make the estimate.

After a number of estimates are made, the operator will begin to get a feel for what they should be, at least in comparison with others he makes. At first, however, it is probably best to think in terms of the 20 to 1 bet as described above. After arriving at the best estimate, the analyst should estimate the confidence limits by adjusting them until he is indifferent to whether he takes the inside or the outside bet (Figure A.7-1).

In some cases, there may be some theoretical or experimental basis for estimating uncertainty. For example, the values of the treatment efficacy, R_{in}, cannot be greater than 1. Therefore, if the best estimate is 0.5, the uncertainty should not be greater than ± 0.5, ±100%, or U = 2 (all almost equivalent ways of expressing the uncertainty). In another case, it may be known experimentally that most rivers have similar velocities of flow under average conditions. Since downstream distances can be measured rather accurately, the transit time can be estimated almost as well as the velocity, say to a factor of 2. If one allows additional concern for turbulent delays, this might be increased to U = 3.

If an uncertainty is thought of in terms of a percentage, P, the nearly equivalent uncertainty factor is

$$U = 1 + \frac{P}{100}$$

for relatively small P (less than 50%).

It is desirable to have all data estimators assign relatively similar uncertainty factors to similar types of data, and to be consistent among data types of differing typical uncertainty. To assist in this calibration, suggested default values for uncertainties in several variables are cited in Annex A.B. These may be changed as experience accumulates.

A.7.1.4 Uncertainty Propagation

The basic idea behind uncertainty propagation from basic input variables to aggregated hazards was described in Section A.2.4, expecially in Figure A.2-9. In principle, a two-fold uncertainty in an input variable could produce exactly a two-fold uncertainty in an aggregate hazard estimate, or much more or much less, depending on the uncertainty in the other variables and the way in which all the variables enter the equation for hazard. Also in principle, the distribution for the aggregate hazard could be exactly predicted if the distributions of all the input variables were known.

In practice, input uncertainties are almost always subjective, the underlying "distributions" are assumed rather than known, and formal statistical techniques do not apply in any rigorous sense. Furthermore, there is no way of unambiguously "verifying" the uncertainty in a hazard estimate by repeated experiments, since none of the experiments measure that hazard directly. Consequently, we turn to a pseudo-statistical treatment of uncertainty propagation only because trying to estimate the uncertainty in a hazard from the component uncertainties by other means is less likely to give useful insights.

Given the assumption of an underlying statistical distribution (always log-normal for propagation), there are two significant possibilities for propagating uncertainty.

First, we can derive an approximate analytic solution based on the moments (mean and variance) of the distribution. Although this has been done for the simplest formulas, it is extremely difficult to do correctly for the more complex expressions. Thus, even though computation times would be short once the analytic solution were programmed, this was discarded for the allocation methodology.

The remaining method is known as the Monte Carlo method, which offers the advantages of conceptual and programming simplicity, but sacrifices computational speed and offers a greater chance that statistical anomalies will invalidate results.

The Monte Carlo method amounts to a simulation of repeated sets of experiments on the component variables of the aggregate hazards. As shown in Figure A.7-3, the first task is to define the output variable (the aggregate hazard) and its relation to the input variables (source quantity, half-life, flow rates, and so on). Next, a set of random numbers (usually in the range $0 < x < 1$) is selected and a corresponding value for the normal variable (zero mean and unit variance) is generated, one for each input variable. Then, using the best estimate and the uncertainty factor from the data base, the mean and the variance for the log-normal distribution define the sample value for the variable. (This procedure is further diagrammed in Figure A.7-4.)

When sample values for all the variables have been generated, they are combined according to the formula to produce a sample value for the aggregate hazard (output variable). This is repeated several times (N in the figure) to produce a set of sample hazards. Finally, the mean and the variance can be computed by standard formulas:

$$\bar{H} = \frac{1}{N} \sum_{s=1}^{N} H_s$$

$$\sigma_H = \sqrt{\left[\sum_{s=1}^{N} H_s^2 - (\Sigma H_s)^2/N\right] \Big/ (N-1)}$$

where $\bar{H}$ is the mean, the H_s are the sample hazards, σ_H is the standard deviation (square root of the variance), and N is the number of samples.

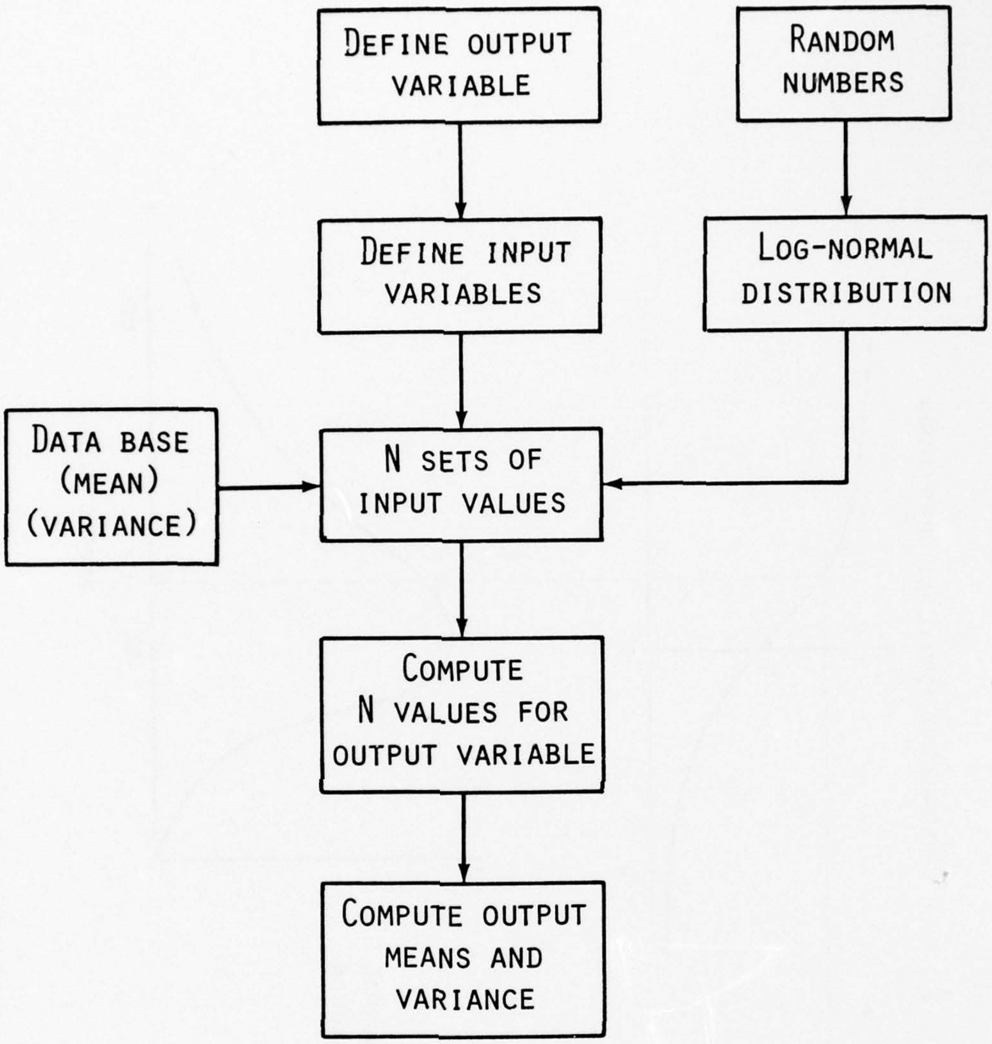


FIGURE A.7-3 MONTE CARLO SIMULATION

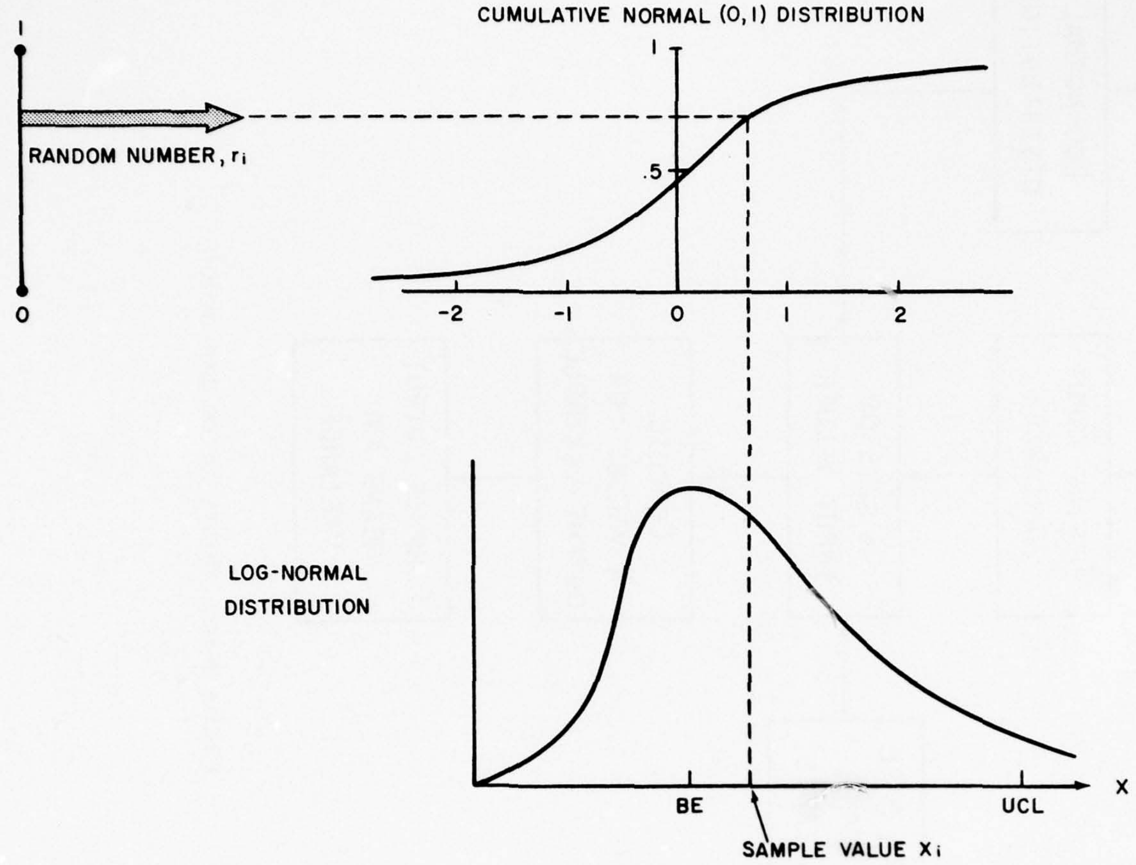


FIGURE A.7-4 GENERATION OF A SAMPLE VALUE FOR A VARIABLE X

In doing this we assume:

- Distributions are log-normal.
- The uncertainty factor defines the 2σ points.
- Different variables are uncorrelated.
- If the same variable enters two or more terms of the aggregate hazard, it assumes the same sample value.

A.7.2 Candidate Research Programs

A research study of any value will reduce the uncertainty in some variable of the hazard estimating system thereby reducing uncertainties in the hazards associated with that variable. The uncertainty in the aggregate hazard (the sum of all hazards) will also be reduced and will be one measure of the study's potential value. Section A.7.2 discusses EPRD candidate programs and their effectiveness in reducing uncertainty.

A.7.2.1 Types of Studies

A research program is defined as a study conducted on a general subject such as acute toxicology in mammals, or environmental chemistry. A research study is one conducted on a specific subject such as environmental chemistry of TNT in water. A project is that part of a study that addresses a specific variable. Many studies address only one variable (environmental chemistry of TNT in water measures the rate constant, λ_{im}, for i = TNT and m = H2O), but some address more than one (epidemiology of HMX measures $S_{im\ell}$ both for cancer--ℓ = C--and for other serious chronic effects--ℓ = CTG). The value of a study includes the values of all its projects.

The general programs of interest to EPRD were discussed in Section A.2.1.2. Table A.7-2 lists codes and names of programs currently defined to be of immediate or potential significance to the allocation methodology. Table A.7-2 also shows the variables associated with the different projects that would be conducted during a specific

Table A.7-2

SUMMARY OF PROGRAM COSTS AND EFFECTIVENESS VALUES
December 1, 1976

Code	Program Title	Variables	Indices[a]		Cost ($)	Uncertainty[b]	Notes[c]
			Fixed	Selected			
EPI	Epidemiology (retrospective cohort study)	Slope of dose-response relation (S)	Effect = cancer in man Effect = chronic toxicity (unspecified) Effect = chronic toxic recoverable	Chemical, medium of exposure	$200,000	* 7 * 10 * 10	One study to look for all three types of effects. Costs from SRI (Holdsworth)
LTM	Lifetime tests in mammals	Slope of dose-response relation (S)	Effect = cancer in man Effect = chronic toxicity (unspecified Effect = chronic toxic recoverable	Chemical, medium = water, groundwater Chemical, medium = air	400,000 450,000	* 7 * 7 * 3	Two or more species, at least two years, look for all three effects. Costs averaged between EPRD and SRI (Liu)
MUT	Ames-type mutagenic assay	Slope of dose-response relation (S)	Effect = cancer in man	Chemical, medium of exposure	1,100	* 25	MCA p.124; no difference for volatiles (SRI-Simmon)
90D	90-day tests in mammals	Slope of dose-response relation (S)	Effect = chronic toxicity (unspecified) Effect = chronic toxic recoverable	Chemical, medium = water, groundwater Chemical, medium = air	45,000 50,000	* 10 * 7	Look for both effects; costs averaged between EPRD and SRI (Dilley)
ATM	Acute toxicity in mammals	Slope of dose-response relation (S)	Effect = acute toxicity in man	Chemical, medium = water, groundwater Chemical, medium = air	1,500 2,000	* 3	Not applicable to chronic effects; costs averaged between MCA p.124 and EPRD; oral and dermal LD_{50}
CAT	Chronic aquatic toxicity	Slope of dose-response relation (S)	Effect = chronic toxicity in fish	Chemical, medium = water	50,000	* 2	Two or more species; costs average of EPRD and SRI (Liu)
AAT	Acute aquatic toxicity	Slope of dose-response relation (S)	Effect = chronic toxicity in fish Effect = acute toxicity in fish	Chemical, medium = water	20,000	* 7 * 2	EPRD Phase II protocol Cost + effectiveness EPRD
SAT	Screening aquatic toxicity	Slope of dose-response relation (S)	Effect = chronic toxicity in fish Effect = acute toxicity in fish	Chemical, medium = water	8,000	* 15 * 4	EPRD Phase I protocol Cost + effectiveness EPRD (more than preliminary screening)
AFS[d]	Aquatic field survey	Hazard for plant effluents (H)	Medium = water Location = fish	Location	75,000	* 5	Study addresses more than just fish, but not human; interpretation of effectiveness to cost ratio is unclear
ECH	Environmental chemistry, includes rate constants for chemical and biochemical processes and physical transfers	Rate constant for chemical disappearance (LMD) Diffusion rate constant (D)	Medium = water Medium = air or groundwater[e] Medium = groundwater	Chemical Chemical Chemical	60,000 40,000 40,000	* 3 * 3 + 30	Includes biodegradation - costs from SRI study for EPA. Determination of LMD assists in estimating D in absence of sampling

Table A.7-2 (Concluded)

Code	Program Title	Variables	Indices[a]		Cost ($)	Uncertainty[b]	Notes[c]
			Fixed	Selected			
SAM[d]	Sampling concentrations	Concentration in medium (C)	Medium = water Medium = air Medium = groundwater	Chemical, location	$ 30,000 40,000 45,000	* 3 * 3 * 3	Attempts to predict annual averages at several (~5) population centers near location; also gives indirect information for LMD or D for estimating unsampled concentrations
SSM	Source strength measurement	Source discharge rate (Q)	Medium = water Medium = air Medium = groundwater	Chemical, location	15,000 30,000 20,000	+ 25 * 2 * 5	Quantifying discharge for known pollutants; water discharge times concentration, air concentration in stacks, water concentration in ponds, and leak rate, etc.
ANT[d]	Development of analytic techniques	Concentration in medium (C)		Chemical, medium	10,000	* 6	Applicable only if SAM or SSM is planned but C expected to be below detectable limits; add to cost of SAM or SSM; change uncertainty
CHI	Identification of new chemical species at a location	Source discharge rate (Q)	Chemical = unknown location	Location, medium	20,000	* 5	Could be combined with SSM, but typically requires different techniques
HYD[d]	Hydrology of river system	Low volume flow rate (SMF) Transit time (SMT)	Population type = fish Effect = ATF Population types = humans and fish	Location	25,000	* 2 + 10	Better data on low-flow dilution at fish concentration areas and transit time to populations at risk through dye dispersion, etc
TRT	Treatment efficacy	Fraction remaining after treatment (R)	Population type = human	Chemical	15,000	* 2	EPRD cost estimate
HG1	Hydrogeology (velocities)	Aquifer flow rates (SMV)	Medium = groundwater	Location	100,000	* 1.5	Injection/withdrawal studies
HG2	Hydrogeology (diffusion)	Diffusion rate constant (D) Source discharge rate (Q)	Medium = groundwater	Location, chemical	25,000	+ 10 * 3	Sampling at several existing wells and regression analysis; incremental cost per chemical
VAL[d]	Relative valuation of effects in populations	Values of effects (V)	All effects on all population types		10,000	* 3	A sampling of opinion and research on values; would affect total hazard over all chemicals and locations

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[a] Hazards would be summed over all indices not specified to compute hazard-uncertainty. Some programs address several variables.

[b] The uncertainty in the variable after the program: * for multiplicative uncertainty factor, + for ± percent uncertainty.

[c] Documentation of program cards would be specific; e.g., MCA = Data from Manufacturing Chemists Association, 1975.

[d] Definition of this program's parameters needs further study.

study from the program area. However, existing methodology cannot evaluate all of the listed programs because of conceptual difficulties; possibilities for resolving these difficulties are discussed in the recommendations, Section A.8.2.5. These difficult programs are indicated by the symbol d.

Each program is considered to have a standard basic protocol that can be modified to fit unique circumstances for a specific study. Many such protocols are already standardized at EPRD, but some are newly defined here, and may be modified before implementation.

The correspondences between the programs defined in Table A.7-2 and those defined by EPRD are shown in Table A.7-3. Since most of the programs have relatively well-established protocols at EPRD, only the exceptions are discussed here.

Epidemiology (EPI) is a study of mortality or morbidity in humans exposed to a chemical agent. Either a retrospective study can be done which looks only at histories of illness in people who have already been exposed, or a prospective study, which follows people who are or were exposed to determine further illness. Epidemiology can concentrate on people with disease to determine what factors were involved, or examine an entire exposed population, recording both illness and freedom from it. The epidemiology protocol proposed here is relatively simple: a retrospective examination of people exposed to a known chemical agent, and an attempt to determine their dose levels. All chronic effects, including cancer, would be noted. Mortality and morbidity would both be analyzed.

Environmental chemistry (ECH) is a study of the breakdown and conversion of primary pollutants into other compounds, but should also include study of the physical transfers of a pollutant from one medium to another. Among the phenomena to be studied are: hydrolysis, oxidation, photolysis and photo-oxidation, biodegradation, volatility (evaporation), sorption to sediments, deposition (wet and dry) from air, and removal by percolation through soils. Identification of the major breakdown products should also be accomplished.

Table A.7-3

CORRESPONDENCES BETWEEN SRI AND EPRD DEFINITIONS OF RESEARCH PROGRAMS

SRI Code	EPRD Definition	Notes
EPI	--	Not currently done
LTM	Mammalian Toxicology, Phase III	--
MUT	--	Included in Phase I Mammalian Toxicology
90D	Mammalian Toxicology, Phase II	--
ATM	Mammalian Toxicology, Phase I	Excluding mutagenesis
CAT	Aquatic Toxicology, Phase III	--
AAT	Aquatic Toxicology, Phase II	--
SAT	Aquatic Toxicology, Phase I	--
AFS	Aquatic Field Survey	--
ECH	--	Newly defined
SAM	--	Not standardized
SSM	--	Sometimes as part of problem definition
ANT	--	May be part of chemical characterization
CHI	Chemical Characterization	EPRD usually includes identification of breakdown products here
HYD	--	Included as part of Problem Definition
HG1	--	
HG2	--	
TRT	--	Not currently done
VAL	Valuation	Not currently done
--	Phytotoxicology	Program not yet defined by SRI

Sampling (SAM) is an identification of actual pollutant concentrations in environmental media. Although any sampling points can be used, a sampling program is more meaningful if related to the populations exposed to the pollutant being sampled. Sufficient samples should be collected and analyzed (by standard methods) to adequately characterize the annual average and peak concentrations.

Development of Analytic Techniques (ANT) usually accompanies another program like SAM, SSM, or CHI, when existing analytic techniques fail to properly identify and distinguish chemicals at the concentration levels found. By definition, this research cannot be standardized.

Treatment Efficacy (TRT) is a study of the relation of concentration in finished drinking water to that in raw source water for various water treatment technologies. Either laboratory simulations or measurements at operating facilities could be considered.

Valuation (VAL) entails a study to determine the attitudes of decision makers and their public constituency regarding the relative importance among all of the known effects of Army chemicals. It would probably include paired comparisons among various combinations of effects as well as comparison with economic impacts of several types. This would probably be a one-time study.

A.7.2.2 Relating Studies to Variables in the Hazard Model

Operation of the allocation methodology to evaluate one study against another requires that the study reduce the uncertainty in one or more input variables of the hazard estimating system. Although a given study may in fact give a great deal more subjective information, it is the objective measurement of the values of these variables that is important as far as the allocation model is concerned. The variables that are affected by each type of study (program) are shown in Table A.7-2.

Unfortunately, it is often difficult to define a study in terms of specific model variables. For example, aquatic field surveys are designed to determine whether or not an ecological problem exists near an Army facility, and to state, insofar as possible, the magnitude and distribution of the problem. Much less is done to identify the relationship of the problem to concentrations of specific chemicals. In fact, it may be misleading to try to do so, because it is the aggregate effects of all environmental stresses that is being observed. Currently, it is assumed that the best way of relating an aquatic field survey to the hazard model is through the aggregate hazard estimate for all effects to fish at a given location (facility). However, this hazard clearly does not adequately express damage to invertebrates, aquatic vegetation, and so on. Moreover, the appropriate reduction in uncertainty is not understood, and the computational problems are unsolved.

Similarly, it is reasonably clear that sampling and the development of analytic techniques both act to reduce uncertainty about the concentration of pollutants to which various populations are exposed. However, such concentrations are usually not direct inputs to the model but are instead calculated intermediate results. Difficulties remain in specifying how the model is to evaluate the substitution of a more accurate, measured value for a calculated one.

The valuation study is a final example of difficulties in defining the proper variables affected. Clearly, the relative valuation of one effect in comparison with all the others is a very sensitive parameter of the allocation methodology. The variables affected are all the V's, but what aggregate hazard should be used? Since the study would probably include all effects in all exposed populations, the aggregate hazard could well be the total hazard for all effects at all locations from all chemicals. Even so, the question of how much uncertainty reduction would be achieved by such a study is unanswered.

A number of EPRD current or potential program areas have been excluded from the analysis for different reasons. Some of these programs will be evaluated easily by the methodology once enough data and hazard models are developed, for example other kinds of toxicology, livestock toxicology, and terrestrial field surveys. Other programs, such as determination of populations-at-risk or more accurate measurements of exposure factors like the breathing rate, are unlikely to be defined as being within EPRD's mandate. Finally, some EPRD programs, such as problem definition studies, are done essentially by direction and have results that cannot be easily anticipated or evaluated.

A.7.2.3 Cost and Effectiveness of Programs

As outlined in Section A.2.4, the value of research study lies in its ability to reduce uncertainty without incurring excessive costs. Some studies will cost more than anticipated and/or produce less than they promised. However, the allocation methodology operates before a study is initiated and deals in anticipated costs and uncertainty reductions.

Consequently, many studies belonging to a given program area are assumed to have identical costs and identical results at the time of their selection. For example, there is little a priori reason to expect that the cost and effectiveness of an environmental chemistry study on tetracene would differ substantially from those for a similar study on cyclohexanone, until preliminary data gathering and screening experiments were well under way. Therefore, study costs and uncertainty reduction are considered to be identical for all studies in a given program area unless obvious differences exist, as shown in Table A.7-2. The particular environmental medium contaminated is one of the most obvious discriminations to be made, since the medium affects both the route of exposure (inhalation toxicology is usually more expensive than ingestion toxicology) and the processes operating (biodegradation is relatively unimportant in air).

Effectiveness of a program is as significant as cost. Different projects within a study can have vastly different effectiveness. For example, acute aquatic toxicity tests provide direct information on acute effects in fish, and result in relatively low uncertainties. These tests also provide some information on pollutant levels at which chronic effects in fish are likely to be insignificant, but with much less accuracy. Such differences are reflected in Table A.7-2.

Cost is measured simply in terms of the anticipated funds (in dollars) required to complete a study on a specific subject, during the next allocation cycle.

Uncertainty reduction (that is, effectiveness) is measured in terms of the uncertainty in the variables expected after the study is complete. (This implies, of course, that the study will interpret the data with respect to the variable in question and will give some indication of its reliability.) It is assumed that this subsequent (posterior) uncertainty is independent of the prior uncertainty in the variable; therefore, the effectiveness of the program can be expressed in terms of certainty to be achieved rather than reduction of previous uncertainty. This assumption permits specification of a study's effectiveness without knowing the details of the current state of knowledge as expressed in the variable uncertainties, contained in the data base. Of course, for some studies this assumption is marginally in error. For example, a sampling study with n samples would show no improvement in uncertainty if a previous sample of n had been taken under this assumption. In reality, a small further reduction in uncertainty, roughly proportional to $\sqrt{2}$, would be achieved.

Most subsequent uncertainty values will be expressed in terms of an uncertainty factor, U. It is also possible to specify them in terms of a percentage uncertainty, P. In this case, the computer program will reexpress them in terms of multiplicatively symmetrical ("log-normal") uncertainties. Uncertainties should not be expressed as absolute values, because the outcome of the experiment cannot be predicted but is assumed to be equal to the prior best estimate of the variable in question.

A.7.2.4 Status of Programs

The EPRD maintains a record of the status of existing and potential studies, which discriminates among studies that are completed, under way, planned, candidates for approval, and premature. The last

Table A.7-4

STATUS OF EPRD RESEARCH PROGRAMS
11/29/76

													RMA	SSM							
		EPI	LTM	MUT	90D	ATM	CAT	AAT	SAT	ECH	ANT	TRT	HG2	RAD	VOL	HOL	JOL	SUN	LCY	PBA	RMA
Nitroglycerin	NG	5*	3	3	4	4	4	4	4	1		1	7	3	7	7	7	7	7	7	7
1,3-Dinitroglycerin	13D	0	0	3	1	4	0	0	1	1		1	7	3	7	7	7	7	7	7	7
1,2-Dinitroglycerin	12D	0	0	3	1	4	0	0	1	1		1	7	3	7	7	7	7	7	7	7
1-Mononitroglycerin	1MG	0	0	3	1	4	0	0	1	1		1	7	3	7	7	7	7	7	7	7
2-Mononitroglycerin	2MG	0	0	3	1	4	0	0	1	1		1	7	3	7	7	7	7	7	7	7
Trinitrotoluene	TNT	4	1	3	3	4	1	3	4	1		1	7	4	4	4	4	7	7	7	7
2,6-Dinitrotoluene	26D	0	0	3	0	1	7	7	7	1		1	7	0	4	7	0	7	7	7	7
2,4-Dinitrotoluene	24D	0	0	4	0	1	7	7	7	1		1	7	0	4	7	0	7	7	7	7
4-Amino-2,6-dinitrotoluene	4AD	0	0	3	1	4	7	7	7	1		1	7	0	4	7	0	7	7	7	7
2-amino-4,6-dinitrotoluene	2AD	0	0	3	1	4	7	7	7	1		1	7	0	4	7	0	7	7	7	7
Cyclotetramethylene tetranitramine	HMX	5*	7	1	7	4	7	7	4	1		1	7	7	7	4	7	7	7	7	7
Cyclotrimethylene trinitramine	RDX	5*	3	1	4	4	3	4	4	2		1	7	7	7	4	7	7	7	7	7
Cyclohexanone	CHX	0	0	1	0	1	0	0	1	1		1	7	7	7	4	7	7	7	7	7
Hexamine	HEX	5*	0	1	0	1	0	0	1	1		1	7	7	7	1	7	7	7	7	7
Octahydro... S-tetramine	SEX	0	0	1	0	1	0	0	1	1		1	7	7	7	1	7	7	7	7	7
Nitroguanidine	NGU	0	0	1	0	1	0	0	1	1		1	7	1	7	7	7	0	7	7	7
O-Nitrodiphenylamine	NDP	0	0	1	0	1	0	0	1	1		1	7	3	7	7	7	7	7	7	7
White phosphorus	WPH	0	0	3	1	4	4	4	4	1		1	7	7	7	7	7	7	7	4	7
Trinitroresorcinol	TNR	0	0	1	0	1	0	0	0	1		1	7	7	7	7	7	7	1	7	7
Tetracene	TZ	0	0	1	0	1	0	0	1	1		1	7	7	7	7	7	7	1	7	7
Lead styphnate	PBS	0	0	1	0	1	0	0	0	1		1	7	7	7	7	7	7	1	7	7
Pentaerythritol tetranitrate	PET	0	0	1	0	1	0	0	0	1		1	7	7	7	7	7	7	1	7	7
Tetranitromethane	TNM	1	1	4	3	4	7	7	7	1		7	7	0	7	7	0	7	7	7	7
Nitromethane	NM	0	0	1	0	1	7	7	7	1		7	7	7	7	1	7	7	7	7	7
Methyl nitrate	MM	5*	0	4	1	4	7	7	7	1		7	7	7	7	1	7	7	7	7	7
Mononitrotoluenes	MNT	0	0	4	1	4	7	7	7	1		7	7	0	1	7	0	7	7	7	7
Thiodiglycol	TDG	0	0	3	3	4	0	0	1	1		1	1	7	7	7	7	7	7	1	7
Lewisite oxide	LWØ	0	0	3	3	4	0	0	1	1		1	6†	7	7	7	7	7	7	1	1
Methylphosphonic acid	MPA	0	0	3	3	4	0	0	1	1		1	1	7	7	7	7	7	7	7	1
Isopropylmethyl phosphonate	IMP	0	0	3	3	3	0	0	1	1		1	1	7	7	7	7	7	7	7	1
Diisopropylmethyl phosphonate	DMP	0	1	4	4	4	7	7	4	1		1	4	7	7	7	7	7	7	7	4
Chlorates	CHL	0	1	3	4	4	0	0	1	1		1	4	7	7	7	7	7	7	7	1
Dicyclopentadiene	DPD	1	1	4	4	4	7	7	4	1		1	4	7	7	7	7	7	7	7	4

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*Case studies. †As arsenic.

Table A.7-4 (Concluded)

		SAM-H20								SAM-AIR				SAM-GWT	
		RAD	VOL	HOL	JOL	SUN	LCY	PBA	RMA	RAD	VOL	HOL	JOL	PBA	RMA
Nitroglycerin	NG	4	7	7	7	7	7	7	7	7	7	7	7	7	7
1,3-Dinitroglycerin	13D	0	7	7	7	7	7	7	7	7	7	7	7	7	7
1,2-Dinitroglycerin	12D	0	7	7	7	7	7	7	7	7	7	7	7	7	7
1-Mononitroglycerin	1MG	0	7	7	7	7	7	7	7	7	7	7	7	7	7
2-Mononitroglycerin	2MG	0	7	7	7	7	7	7	7	7	7	7	7	7	7
Trinitrotoluene	TNT	4	2	4	4	4	7	7	7	7	7	7	7	7	7
2,6-Dinitrotoluene	26D	0	2	7	0	7	7	7	7	7	7	7	7	7	7
2,4-Dinitrotoluene	24D	0	2	7	0	7	7	7	7	7	7	7	7	7	7
4-Amino-2,6-dinitrotoluene	4AD	0	7	7	0	7	7	7	7	7	7	7	7	7	7
2-Amino-4,6-dinitrotoluene	2AD	0	7	7	0	7	7	7	7	7	7	7	7	7	7
Cyclotetramethylene tetranitramine	HMX	7	7	4	7	7	7	7	7	7	7	7	7	7	7
Cyclotrimethylene trinitramine	RDX	7	7	4	7	7	7	7	7	7	7	7	7	7	7
Cyclohexanone	CHX	7	7	1	7	7	7	7	7	7	7	1	7	7	7
Hexamine	HEX	7	7	1	7	7	7	7	7	7	7	7	7	7	7
Octahydro... S-tetramine	SEX	7	7	1	7	7	7	7	7	7	7	7	7	7	7
Nitroguanidine	NGU	0	7	7	7	0	7	7	7	7	7	7	7	7	7
O-nitrodiphenylamine	NDP	4	7	7	7	7	7	7	7	7	7	7	7	7	7
White phosphorus	WPH	7	7	7	7	7	7	4	7	7	7	7	7	0	7
Trinitroresorcinol	TNR	7	7	7	7	7	0	7	7	7	7	7	7	7	7
Tetracene	TZ	7	7	7	7	7	0	7	7	7	7	7	7	7	7
Lead styphnate	PBS	7	7	7	7	7	0	7	7	7	7	7	7	7	7
Pentaerythritol tetranitrate	PET	7	7	7	7	7	0	7	7	7	7	7	7	7	7
Tetranitromethane	TNM	7	7	7	7	7	7	7	7	0	7	7	7	7	7
Nitromethane	NM	7	7	7	7	7	7	7	7	7	7	1	7	7	7
Methyl nitrate	MM	7	7	7	7	7	7	7	7	7	7	1	7	7	7
Mononitrotoluenes	MNT	7	7	7	7	7	7	7	7	0	1	7	1	7	7
Thiodiglycol	TDG	7	7	7	7	7	7	1	7	7	7	7	7	0	0
Lewisite oxide	LW0	7	7	7	7	7	7	1	7	7	7	7	7	0	6*
Methylphosphonic acid	MPA	7	7	7	7	7	7	7	7	7	7	7	7	7	1
Isopropylmethyl phosphonate	IMP	7	7	7	7	7	7	7	7	7	7	7	7	7	1
Diisopropylmethyl phosphonate	DMP	7	7	7	7	7	7	7	7	7	7	7	7	7	4
Chlorates	CHL	7	7	7	7	7	7	7	7	7	7	7	7	7	4
Dicyclopentadiene	DPD	7	7	7	7	7	7	7	7	7	7	7	7	7	4

		CHI				
		H20	AIR	GWT	HYD	HGl
Radford AAP	RAD	1	1	7	1	7
Volunteer AAP	VOL	1	1	7	2	7
Holston AAP	HOL	1	1	7	1	7
Joliet AAP	JOL	1	1	7	1	7
Sunflower AAP	SUN	0	0	7	0	7
Lake City AAP	LCY	1	1	7	1	7
Pine Bluff Arsenal	PBA	1	1	1	1	1
Rocky Mt Arsenal	RMA	1	7	1	1	4

Key:
0 - inappropriate pending other studies
1 - candidate for current budget
2 - scheduled to begin
3 - in progress
4 - completed
5 - inconclusive
6 - special conditions
7 - not applicable

Negative integers: Further consideration inappropriate because of regulatory action.

*As arsenic.

category incorporates studies that should not begin before other studies are complete or before certain Army actions or decisions have been taken. Only studies that have not been completed, started, or planned, and are not premature, are candidates for current funding and therefore need to be evaluated by the allocation methodology.

A snapshot (as of late November 1976) of the status of EPRD programs--identified by program code--is shown in Table A.7-4. In addition to the five categories already discussed (codes 0-4), there are codes for three others. Code 5 is used for studies that have been done but for some reason were unsatisfactory or inconclusive. These studies are candiates for repetition, but special definitions of cost and effectiveness may be required. Code 6 is used for studies that were done under special conditions. For example, a sampling study may have measured arsenic when Lewisite oxide was the pollutant of real concern. In this case, further validation and interpretation may be required, but a full-blown study may not be necessary. Code 7 indicates studies that are currently assumed not to be applicable. For example, if a pollutant is not discharged from a given facility, a sampling program at that site would not be applicable. Finally, a negative code shows the status as above, but specifies that the study is not a candidate because the regulatory decision has already been made.

The program status should be updated continuously as studies are planned, started, completed, or as other conditions change. In particular, it should be thoroughly checked before each operation of the allocation methodology, so that no inappropriate studies are evaluated.

A.7.3 Reduction of Hazard Uncertainty

The keys to the allocation methodology are first, the selection of the hazards (six-subscript) that go into an aggregate hazard and second, the way that the uncertainty in the aggregate hazard is reduced through reduction in variable uncertainty achieved by a given study. The basic ideas behind these keys were presented in Section A.2.4; this section simply gives more detail.

A.7.3.1 Uncertainty in a Variable Prior and Subsequent to a Study

Each project in a study measures the value of a variable from the hazard estimating system. Let this general variable be X. Before a study is undertaken, the value of the variable has been estimated, from a previous study, from theoretical considerations, from similarity to other measured values, or from a default value. Let this best estimate be $\hat{X}$. At the same time, the current, or prior, uncertainty, is estimated--usually subjectively--based on the perceived reliability of the information behind the estimate. Ordinarily, the uncertainty estimate will increase from measured to default values. Let the uncertainty be expressed in terms of the "variance" in the value estimate, σ_X^2, or its "standard deviation," σ_X.

Since a basic log-normal underlying distribution is assumed, the most convenient way of expressing uncertainty is by the uncertainty factor, U_X. Since this factor relates to the 95% confidence limits, which are two standard deviations from the mean, and the distribution is logarithmic,

$$\sigma_X \approx \frac{1}{2} \ln U_X \quad .$$

For uncertainties expressed in percentage terms, P_X, the approximation

$$U_X \approx 1 + P_X/100$$

is used.

A similar procedure is used for projecting the hazard uncertainty expected after a study is complete. The projections of subsequent uncertainties are based on an assumed similarity in reliability between the proposed study and studies on different subjects. For example, the subsequent standard deviation in the rate constant for HMX would be assumed to be the same as for TNT measured in a completed environmental chemistry study. Let the subsequent standard deviation in X be σ_X.

It is important to reiterate that the best estimate of the subsequent distribution, $\hat{X}'$, is equal to that for the prior distribution, $\hat{X}$, because otherwise the analyst would have made a better prior estimate.

However, a significant feature of log-normal distributions is that the mean, $\bar{X}$, is not equal to the best estimate but is in fact given by

$$\bar{X} = \hat{X}\, e^{\sigma_X^2/2}$$

This implies that the mean of the subsequent distribution will not be equal to that of the prior; if σ_X decreases, so will $\bar{X}$.

A.7.3.2 Corresponding Uncertainty in Aggregate Hazard

Section A.7.1 described in general terms how an uncertainty in a variable X can be propagated to an aggregate hazard uncertainty H when H is a function of X. This H is generalized in the sense that it can be any additive combination of six-subscript hazards, so long as the variable X is contained in each of them. In fact, the proper aggregate hazard H to use in the allocation analysis of a specific project on variable X is that which combines all of the six-subscript hazards that contain X and no others.

Notice further that a "variable" in this context is itself defined by specific subscripts. That is, the variable $S(i = TNT, m = H2O, \ell = C)$ is different from the variable $S(i = NG, m = H2O, \ell = C)$. Therefore, the appropriate aggregate hazard to use when evaluating a project that will determine the slope of the dose response relation for cancer from TNT in water is (since each term contains the former S)

$$H = \sum_{j,n,k} H_{TNT,\, j,\, H2O,\, n,k,C} \quad .$$

H thus includes all hazards with $i = TNT$, $m = H2O$, and $\ell = C$, but no others. The procedure for defining the aggregate hazard for a given project is shown in Figure A.7-5

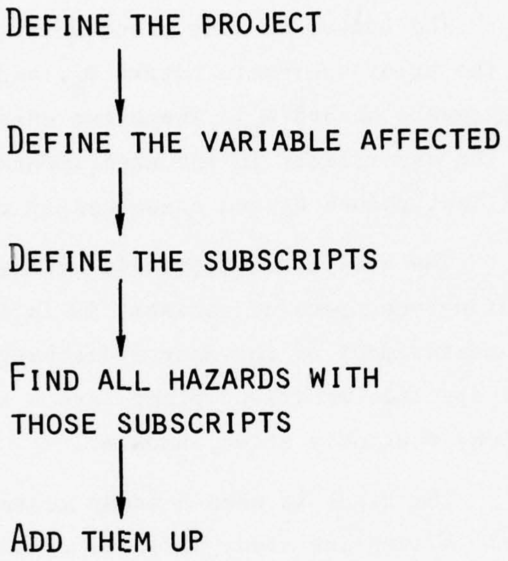

FIGURE A.7-5 DEFINING THE AGGREGATE HAZARD

The identical aggregate hazard is used for both the prior and the subsequent case. All uncertainties are also the same before and after the project except that for the variable measured. The Monte Carlo method is used to propagate uncertainties to the aggregate hazard in both cases. Uncertainties in all variables are used in this propagation, but only that for the variable selected changes from the prior to the subsequent case.

The output of this process is two estimates: the standard deviation of the prior aggregate hazard σ_H, and the standard deviation of subsequent aggregate hazard σ_H'. These two uncertainty estimates differ only because the uncertainty in the experimental variable, X, has changed. Only projects that reduce σ_X and consequently reduce σ_H should be performed.

The analysis is entirely straightforward when only one project measuring one specific variable is included in a study. An example is the measurement of the source discharge rate of a specific chemical at a specific munitions plant into a specific medium. Two kinds of complications routinely arise, however.

The first is when a study measures several variables of the same type. A sampling study measures concentration, C, of a specified chemical, i, around a specified location, j, in a specified medium, m, for <u>all</u> groups, k, of a population type n. Thus the variables measured can be represented by $C_{ijmn.}$, where the . indicates that all values for k are affected. If there are four different k's, there are four different variables affected, with k = 1, 2, 3, or 4. The aggregate hazard in this situation should be the sum of all six-subscript hazards that contain <u>any</u> of the four variables, but no others. Symbolically,

$$H = \sum_{k,\ell} H_{ijmnk\ell}$$

in which i, j, m, and n are all specified, and the sum runs over k, to account for the four different variables, and over ℓ, to account for the improvement in knowledge of the hazards from all effects. As far as the computer is concerned, it is essential that all subsequent uncertainties for the variables of this type are the same, and are specified in a single project card. By definition, then, a project consists of the measurement of the values of one or more variables of the same type.

The second complication arises when a study involves two different types of variables. For example, the hydrology study measures both river flow rates and transit times. In fact, each of these types of variables is a multiple-variable project in itself because the values are measured for several population group points (different k). In principle, the aggregate hazard should sum all six-subscript hazards that contain any variable of either type with the correct specified subscripts. (In the example of hydrology, these would be the location, j, which specifies the river of interest, and for the flow rates, the population type, n = fish. Currently, however, the computer program can aggregate hazards only for a defined project and the evaluation of a study with two or more projects remains a manual task. Although the procedure is not quite correct, the standard deviations for the projects are simply added to estimate the standard deviation for the study.

In certain cases, a study measures only one type of variable, but the uncertainty reduction to be achieved differs for different subscripts of the variable. Lifetime tests in mammals, for example, appear to give greater certainty about chronic recoverable effects than they do about cancer. In such cases, the study is divided into projects as in the instance of different variable types. A procedure for evaluating by computer all projects in a study is under development.

A.7.3.3 Comparison with Study Cost

As outlined in Section A.2.3, the uncertainties in aggregate hazard are of major concern to regulatory agencies. Reduction of these uncertainties is a direct measure of the benefit of conducting a study. In the allocation methodology, the standard deviations computed by the Monte Carlo procedure are indicative of these benefits:

$$\Delta\sigma_p = \sigma_H - \sigma_H'$$

where H is the appropriate aggregate hazard for a project p. The higher the ratio of this benefit to the cost of a study, the more attractive it is for funding. The index of preference, I_p, for a given project is thus given by

$$I_p = \frac{\Delta\sigma_p}{C_p}$$

where C_p* is the cost of the project.

If several projects are conducted in a study, an index for the study, I_s, can be generated by

$$I_s = \frac{\sum_p \Delta\sigma_p}{\sum_p C_p}$$

(Ideally, $\Delta\sigma_s$ would be used in the numerator instead of the sum.)

A.7.4 Allocation Methodology Operation

About every 6 months, or more often if conditions change markedly, EPRD will operate the allocation methodology to get guidance on preferred studies to be funded.

A.7.4.1 Overview of the Computer Model

The basic computer program flow for AMRDCP (AMRDC Program) is shown in Figure A.7-6. Data for the hazard model and the project cards of the study deck are read and processed. Random numbers are generated and sample values for each variable selected. The aggregate hazard is defined for each project and calculated for the variable uncertainties before and after the project. This is repeated for a preselected number of iterations, the resulting sample hazards are averaged, and the variances and standard deviations are computed. The index of preference (benefit/cost ratio) is computed and output along with other intermediate results.

More detail on the Monte Carlo and aggregate hazard parts of the model are shown in Figures A.7-7 and A.7-8.

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*Not to be confused with C_{ijmnk}, which is a concentration.

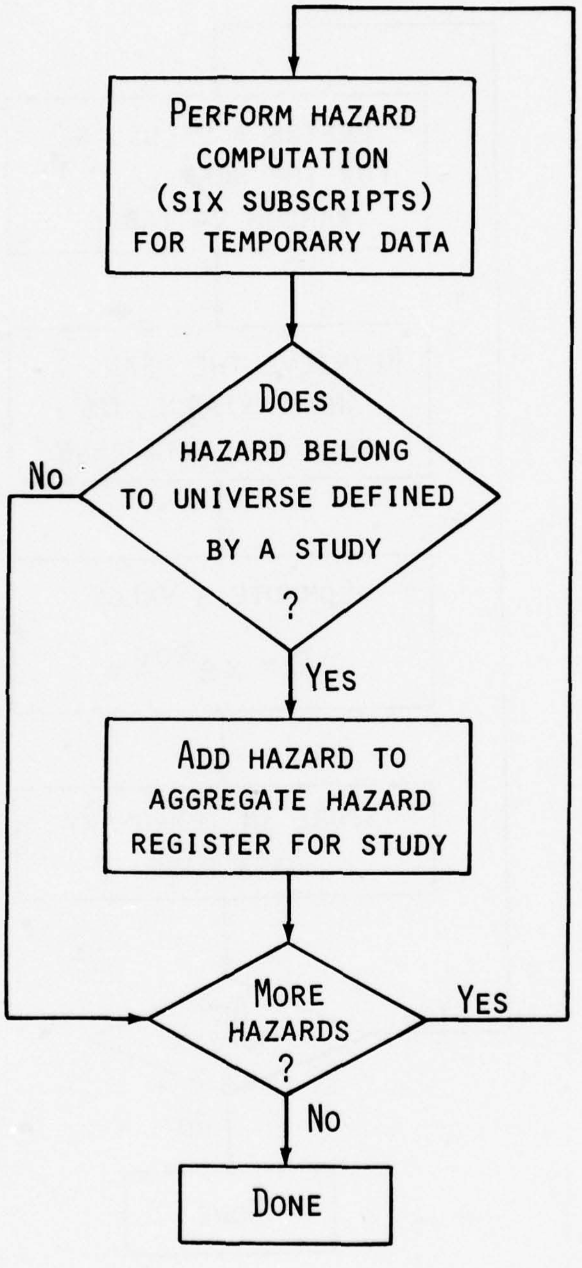

FIGURE A.7-6 ALLOCATION PROGRAM FLOW

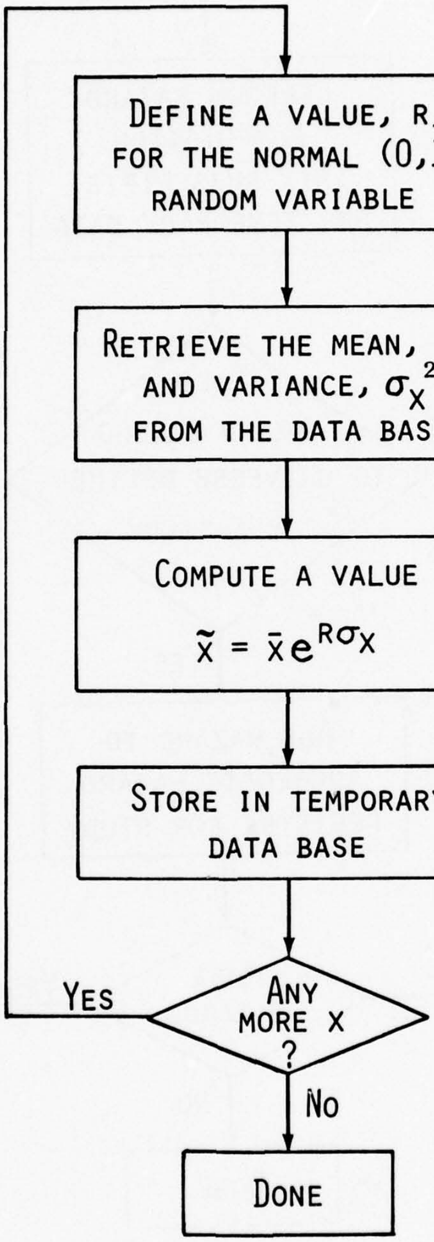

FIGURE A.7-7 MONTE CARLO DETAILS

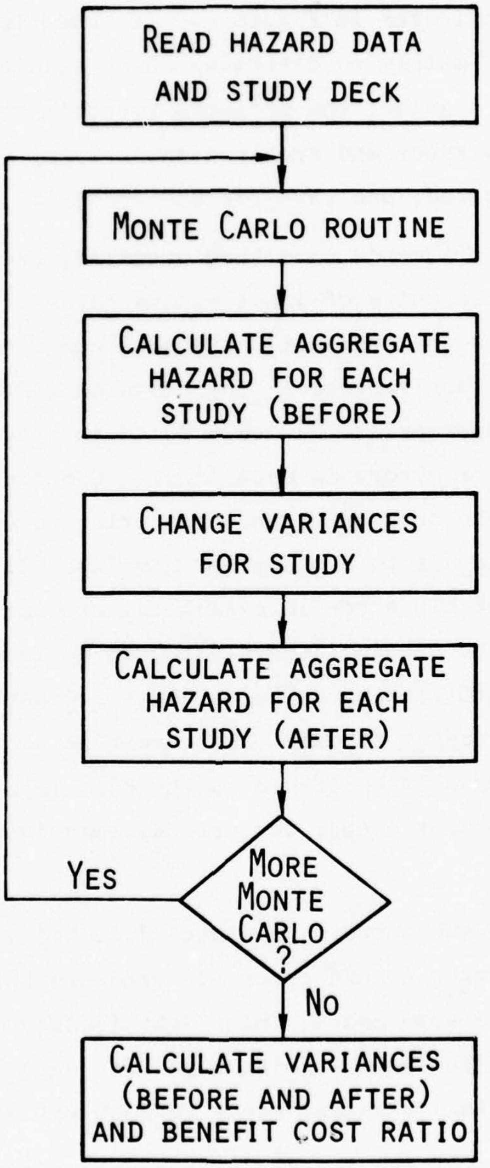

FIGURE A.7-8 AGGREGATE HAZARD DETAILS

A sample output of the allocation model is shown in Figure A.7-9. The values shown are based on test data and should not be considered as actual results.

A.7.4.2 Manual Steps

As indicated in Figure A.7-10, the first step is to review and update the status matrix to determine which studies are candidates. Using Table A.7-2 as a guide, the projects for this study are defined in terms of the variable types and specific subscripts, and data inputs for the computer are prepared, one card for each project.

When all cards have been prepared, they are sorted into groups that fit defined units of input hazard data. (The air, water, and groundwater pollutants are ordinarily run separately to conserve computer storage and run time requirements.) The computer model is then run for each group with the appropriate hazard model data base. First, there are ample opportunities for errors in data input. Sometimes the subsequent uncertainty is equal to or greater than the prior uncertainty, and sometimes hazard data relevant to a study are missing. In the former case, there may be a correctable error in estimating or coding the uncertainty. In the latter case, the missing hazard data can be identified and supplied either from real information or default values. Other errors may relate to the estimation or coding of data that result in abnormally high or low $\Delta\sigma$. These can also usually be traced to the data inputs. The operator then examines the computer output for errors, omissions, and unexpected output.

After such errors have been detected and corrected, the operator should aggregate $\Delta\sigma$ and costs for projects that would be conducted in the same study. In some cases, this might include combining two or more computer-analyzed studies into a joint study for actual funding, for example by authorizing a toxicological study on both TNT and NG.

The resulting indexes of preference are then ranked for presentation to EPRD staff for further checking and elimination. Final studies are selected on the basis of the ranking, subjective considerations, and budgetary limitations.

```
RATIOS OF REDUCTION IN UNCERTAINTY OVER PROG.COST

PROGRAM   VAR   CHE  LOC  MED  POP  PCP  EFF   --------PRIOR--------  ------SUBSEQUENT------  DELTA    PROG.COST  RATIO
-------   ---   ---  ---  ---  TYP  IND  ---     HAZARD       SIGMA      HAZARD       SIGMA    SIGMA    DOLLARS    -------

  ECH     LMD   NG        H20                    126.86      150.05      126.43      155.98       0.*    60000.    0.000
  ECH     LMD   13D       H20                    198.40       40.00      196.89       37.03       3.     60000.     .000
  ECH     LMD   12D       H20                     43.15       46.33       42.95       43.69       3.     60000.     .000
  ECH     LMD   1MG       H20                    267.20      116.01      266.09      116.34       0.*    60000.    0.000
  ECH     LMD   2MG       H20                     28.86       38.77       28.86       38.77       0.     60000.    0.000
  ECH     LMD   TNT       H20                 101458.56    43460.31    81664.92    28165.69   15295.     60000.     .255
  ECH     LMD   26D       H20                   9663.83     8478.66     9663.83     8478.66       0.     60000.    0.000
  ECH     LMD   24D       H20                 780424.83  1100584.08   768032.59  1082693.39   17891.     60000.     .298
  ECH     LMD   4AD       H20                   2063.65     2548.16     2063.65     2548.16       0.     60000.    0.000
  ECH     LMD   2AD       H20                   2794.52     2195.92     2794.52     2195.92       0.     60000.    0.000
  ECH     LMD   HMX       H20                    377.23      317.99      284.01      388.67     129.     60000.     .002
  ECH     LMD   CHX       H20                  75320.12    46849.31    75638.14    47187.13       0.*    60000.    0.000
  ECH     LMD   HEX       H20                       .01         .02         .01         .02       0.     60000.    0.000
  ECH     LMD   SEX       H20                       .75         .93         .75         .93       0.     60000.     .000
  ECH     LMD   NGU       H20                    333.91      455.27      332.97      453.83       1.     60000.     .000
  ECH     LMD   NDP       H20                      0.00        0.00        0.00        0.00       0.     60000.    0.000
```

FIGURE A.7-9   RATIOS OF REDUCTION IN UNCERTAINTY OVER PROGRAM COST

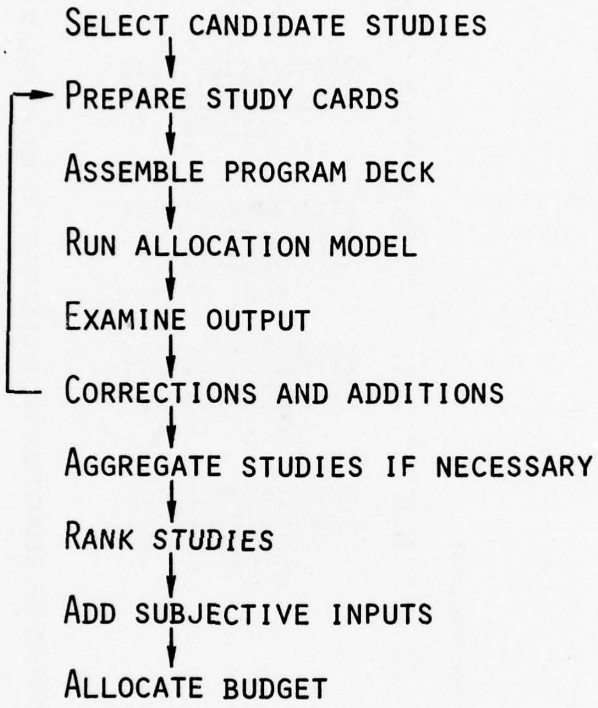

FIGURE A.7-10 STEPS IN OPERATING THE ALLOCATION MODEL

Any new data that become available before the next operation of the methodology are added to the data base (or substituted for outmoded data) before the cycle begins anew.

A.8 INITIAL RESULTS

Section A.8 presents and discusses results obtained from the hazard estimating and ranking system and the allocation methodology by early 1977.

The hazard estimating and ranking system was first exercised by SRI using data assembled by SRI through June of 1976. The outputs of the computer runs were extensively checked and verified against those from a temporary manual system used to generate results for the interim report (April 1976). Since then, the data base has been considerably expanded, revised, and improved, by SRI and especially by EPRD. The results presented here are from the latest approved exercise of the system, either by SRI or EPRD, up to December 31, 1976.

The allocation methodology has been tested and revised several times to eliminate programming and logical errors, and this process is continuing at the time of writing. The results presented here are therefore only illustrative.

A.8.1 Hazard Estimating and Ranking Results

The hazard estimating and ranking system generates hazard estimates from the best estimates of all the input variables for each hazard algorithm. The allocation methodology calculates means and standard deviations for the hazard estimates,* and these can be compared with the best estimates (see Section A.8.2).

A.8.1.1 Pollutants for Ranking

The selection of pollutants and locations of discharge (Army ammunitions plants and arsenals) has already been discussed in Section A.3.

---

*Currently on a linear, or arthmetic, basis; in the future, on a logarithmic, or geometric, basis.

A matrix of Army pollutants by location is shown in Table A.8-1. Civilian chemicals and locations are shown for comparison in Table A.8-2.

A.8.1.2 Hazard-Ranked List

Hazard values were computed from variable data input by HERS and are shown by chemical, ranked from highest to lowest aggregate hazard, in Table A.8-3. The corresponding results for the civilian chemicals are shown in Table A.8-4. Ranking of Army pollutant locations according to the total hazard of all chemicals released from a location is shown in Table A.8-5.

A.8.1.3 Discussion

In examining the hazard-ranked lists and their components, a number of interesting features stand out.

First, the estimated total hazard for all Army chemicals ranked is low, at under $1,000,000 per year. Remember, however, that this total is subject to many caveats, among which are:

- Dollar valuation is controversial both as a technique and as to appropriate values.
- Most of the input data and models are highly uncertain.
- The estimates are best estimates rather than being conservative for standard-setting purposes.

Second, the hazard distribution by chemical ranges over about six orders of magnitude, which can be expected for such a wide variety of chemicals. Thus, only if uncertainties were considerably greater than 100-fold could chemicals in the lower portion of the list move to the top.

Third, the variation from location to location is also marked, and spans over three orders of magnitude.

Fourth, the top-ranked seven pollutants include representatives from each of the three major polluted media: five water pollutants including RDX, nitroglycerin, TNT, and related compounds; methyl

Table A.8-1

ARMY POLLUTANTS AND THEIR LOCATIONS FOR HAZARD RANKING

Pollutant Code	Medium	HOL	JOL	VOL	RAD	LCY	SUN	RMA	PBA
NG	H20				X				
13D	H20				X				
12D	H20				X				
1MG	H20				X				
2MG	H20				X				
TNT	H20	X	X	X	X				
26D	H20	X	X	X	X				
24D	H20	X	X	X	X				
4AD	H20	X	X	X	X				
2AD	H20	X	X	X	X				
HMX	H20	X							
RDX	H20	X							
CHX	H20	X							
HEX	H20	X							
SEX	H20	X							
NGU	H20				X		X		
NDP	H20				X				
WPH	H20								a
TNR	H20					X			
TZ	H20					X			
PBS	H20					X			
PET	H20					X			
TNM	AIR			X	X				
MNT	AIR			X	X				
NM	AIR	X							
MN	AIR	X							
TDG	GWT							X	
LWO	GWT							X	
MPA	GWT							X	
IMP	GWT							X	
DMP	GWT							X	
CHL	GWT							X	
DPD	GWT							X	

---

a - Data incomplete.

Table A.8-2

CIVILIAN CHEMICALS AND THEIR LOCATIONS FOR HAZARD RANKING

Pollutant Code	Medium	Location Name and Code
BNZ	H20	Taft, LA (TFT) Chocolate Bayou, TX (CHB)
NBZ	H20	Gibbsville, NJ (GBT) Beaumont, TX (BMT)
CTC	H20	South Charleston, WV (SCH) Lemoyne, AL (LEM)
VC	AIR	Illiopolis, IL (ILP) Louisville, KY (LVL)
DDM	AIR	Institute, WV (INS) Danville, IL (DVL)

Table A.8-3

ARMY POLLUTANTS RANKED BY HAZARD

Rank	Code	Chemical Name	$/Year Hazard	Medium
1	RDX	RDX	$419,000	H20
2	24D	2,4-Dinitrotoluene	144,000	H20
3	TNT	Trinitrotoluene	115,000	H20
4	CHL	Chlorates	39,000	GWT
5	NG	Nitroglycerin	29,000	H20
6	26D	2,6-Dinitrotolueue	1,900	H20
7	MN	Methyl nitrate	1,900	AIR
8	LWO	Lewisite oxide	1,850	GWT
9	MNT	Mononitrotoluenes	1,800	AIR
10	NGU	Nitroguanidine	1,300	H20
11	TDG	Thiodiglycol	850	GWT
12	TNM	Tetranitromethane	230	AIR
13	2AD	2-Amino-4,6-dinitrotoluene	140	H20
14	4AD	4-Amino-2,6-dinitrotoluene	140	H20
15	13D	1,3-Dinitroglycerin	120	H20
16	TNR	Trinitroresorcinol	110	H20
17	PBS	Lead styphnate	61	H20
18	IMG	1-Mononitroglycerin	56	H20
19	TZ	Tetracene	17	H20
20	DMP	Diisopropylmethylphosphonate	14	GWT
21	12D	1,2-Dinitroglycerin	12	H20
22	MPA	Methylphosphonic acid	9	GWT
23	IMP	Isopropylmethylphosphonate	9	GWT
24	CHX	Cyclohexanone	9	H20
25	NDP	Nitrodiphenylamine	3	H20
26	2MG	2-Mononitroglycerin	1	H20
27	NM	Nitromethane	<1	AIR
28	HEX	Hexamine	<1	H20
29	HMX	HMX	<1	H20
30	SEX	SEX	<1	H20
31	PET	Pentaerythritol tetranitrate	<1	H20
32	DPD	Dicyclopentadiene	<1	GWT
		Total	$750,000	

Table A.8-4

CIVILIAN CHEMICALS RANKED BY HAZARD*

Rank	Code	Chemical Name	$/Year Hazard	Medium
1	DDM	Dichlorodifluoromethane†	75,000,000	AIR
2	VC	Vinyl chloride	14,000,000	AIR
3	NBZ	Nitrobenzene	2,500,000	H20
4	BNZ	Benzene	1,800,000	H20
5	CTC	Carbon tetrachloride‡	17,000	H20

---

*Scaled by production from two locations to all locations.

†May be overestimated by factor of 1,000 because of faulty carcinogenicity rating.

‡May be underestimated by factor of 100 because of faulty evaporation assumption.

Table A.8-5

ARMY LOCATIONS RANKED BY HAZARD

Rank	Location Code	Location	$/Year Hazard
1	HOL	Holston	420,000
2	RAD	Radford	195,000
3	VOL	Volunteer	88,000
4	RMA	RMA	41,000
5	JOL	Joliet	4,700
6	LCY	Lake City	180
7	SUN	Sunflower	150
	Total		750,000

nitrate in air; and chlorates in groundwater. Holston, Volunteer, RMA, and Radford all have at least one pollutant with an estimated hazard in excess of $10,000 per year.

Fifth, several effects contribute to the hazard estimates, including fish kill, cancer in humans, and other human effects. The no-threshold assumption is most important for operation of the system as it currently stands. The system is thus somewhat biased toward routine emissions and average exposure conditions. Treatment of unusual exposure would require a treatment of the likelihood of rare events, and would demand data (or intelligent assumption) as the statistical distribution thereof. Currently, many more default values for noncarcinogenic effects are being developed. This will undoubtedly raise the total estimated hazard, but will have considerably less effect on the hazard ranks. The latter is true because the ranks are much more dependent on differences in exposure than on differences in the estimate of carcinogenic potential, and default values for other effects are expected to have only a moderate spread.

A.8.1.4 Conclusions and Recommendations

The process of designing, implementing, and operating the hazard estimating and ranking system has led the SRI project team to the following conclusions:

(1) A mathematical model of environmental pollution has been constructed that can give significant insights into the relative importance of environmental hazards from different chemicals, sources of pollution, media of discharge, species at risk, effects caused, and so on.

(2) The model indicates that the Army activities considered are probably causing only moderate pollution problems in comparison with those of civilian chemical production.

(3) The model indicates that there are wide differences among chemicals as to hazard posed, and that the hazards occur predominantly in the form of human health effects. The latter conclusion, however, may be in part due to biases inherent in the selection of effects to consider.

(4) The assumption that pollution problems for a given chemical are unique to one environmental medium is often, but not always, true.

(5) Proper consideration of environmental behavior (physical and chemical removal processes, transport phenomena, and so on) is essential for understanding relative hazards.

(6) Many aspects of pollutant hazards, such as ecosystem effects, are currently not sufficiently understood to be modeled successfully.

The following recommendations are offered in connection with the above conclusions:

(1) The hazard estimating and ranking model should be used as a complement to the allocation model in a program of surveillance over Army related pollution problems. The model's output should be examined as one indicator of the pollution abatement activities that could have the highest hazard-reduction potential. However, the information processed by HERS and AMRDCP is too uncertain for it to serve as the sole base for important operational decisions.

(2) Additional input data and models should be developed for HERS and AMRDCP to account for phenomena not currently well-treated. Such activities could be as simple as generating additional default values for already established phenomena or as complex as the development of complete new modules for the system. (Development of an occupational health module is in fact just beginning.)

(3) Attention should be directed to the consideration of expanded research areas for EPRD, such as environmental chemistry (already begun) or epidemiology (done only to a very limited extent).

(4) Some consideration of the model's data needs should be included in the design of research programs, once selected. (The selection of programs is covered in Section A.8.2.)

A.8.2 Allocation Methodology Results

The allocation methodology include all the manual pre- and post-computer steps discussed in Section A.7.4.2, but the heart of the methodology is the computer model AMRDCP derived from HERS, which essentially repeatedly calculates hazards using different Monte Carlo samples from the distributions of input variables. These steps are carried out both for the current situation (prior values of all variables) and for the assumed situation after a research study is completed (subsequent values). The computer prints prior and subsequent hazards for each sample and for each evaluated study. It also prints the mean and standard deviation of the prior hazards by chemical and location. Finally, it prints the summary of prior and subsequent aggregate hazards and their standard deviations for each study, as well as the ratio of the different in standard deviations to the cost of a study, as an index of preference.

A.8.2.1 Candidate Research Programs

The candidate studies used in the first exercise of the allocation model are those coded "1" in the status matrix, Table A.7-4, with the following exceptions:

- Sampling programs (SAM) have not yet been evaluated because they entail measurements of a variable (C_{imjnk}) that was previously calculated.
- Hydrology programs (HYD) have not yet been evaluated because they entail measurement of two variables (SMF and SMT) at several population groups.
- Certain specific studies have not yet been evaluated because all of the appropriate input data have not been generated.

A.8.2.2 Computer Model Output

Sample computer output is shown in Tables A.8-6 and A.8-7 for the hazard summary matrix and the allocation figure of merit, respectively. The data bases involved differed from those for which results were presented in Section A.8.2; hence, the outputs do not compare.

The notation "No value for this program's variable in data base" should suggest either

- that data are missing and should be supplied,
- that the program is not meaningful at present and should be dropped, or
- that the data for evaluating this program are in another file and will be evaluated in a separate run.

The asterisk following 0. in the column labeled "Delta Sigma" indicates a negative value for Delta Sigma. Reasons for this situation are that:

- The prior uncertainty value is less than the value subsequent to the program. These values should be examined to determine if assignments are valid.
- The Monte Carlo simulation is not rapidly convergent.

The second error is more serious. It can be demonstrated that it is possible to generate a negative Delta Sigma even when the subsequent uncertainty

TABLE A.8-6 SAMPLE OUTPUT OF HAZARD SUMMARY MATRIX

```
HAZARD SUMMARIES BY CHEMICAL AND LOCATION FOR

     TSTIB

CHEMICAL         HOLSTON      JOLIET     RADFORD  ROCKY MT A   VOLUNTEER    ALL LOCS

SODIUM CHLOR          0.          0.          0.     139601.          0.     139601.
  ATE OR CHLOR
  ATE SALTS
    STD.DEV.          0.          0.          0.      66850.          0.      66850.

CYCLOHEXANON      75320.          0.          0.          0.          0.      75320.
  E
    STD.DEV.      46849.          0.          0.          0.          0.      46849.

DIISOPROPYL           0.          0.          0.        181.          0.        181.
  METHYLPHOSPH
  ONATE
    STD.DEV.          0.          0.          0.          2.          0.          2.

DICYCLOPENTA          0.          0.          0.        901.          0.        901.
  DIENE
    STD.DEV.          0.          0.          0.       1195.          0.       1195.

HEXAMINE              0.          0.          0.          0.          0.          0.
    STD.DEV.          0.          0.          0.          0.          0.          0.

HMX                 377.          0.          0.          0.          0.        377.
    STD.DEV.        518.          0.          0.          0.          0.        518.

ISOPROPYL ME          0.          0.          0.          6.          0.          6.
  THYLPHOSPHON
  ATE
    STD.DEV.          0.          0.          0.          8.          0.          8.

LEWISITE OXI          0.          0.          0.        298.          0.        298.
  DE
    STD.DEV.          0.          0.          0.        389.          0.        389.

METHYLPHOSPH          0.          0.          0.         53.          0.         53.
  ONIC ACID
    STD.DEV.          0.          0.          0.         11.          0.         11.

NITROGUANIDI          0.          0.        334.          0.          0.        334.
  NE
    STD.DEV.          0.          0.        455.          0.          0.        455.

NITROGLYCERI          0.          0.        127.          0.          0.        127.
  N
    STD.DEV.          0.          0.        150.          0.          0.        150.

RDX                 964.          0.          0.          0.          0.        964.
    STD.DEV.        175.          0.          0.          0.          0.        175.

SEX                   1.          0.          0.          0.          0.          1.
    STD.DEV.          1.          0.          0.          0.          0.          1.

THIODIGLYCOL          0.          0.          0.     624087.          0.     624087.
    STD.DEV.          0.          0.          0.     876696.          0.     876696.

2,4,6 TRINIT      72849.       1146.       7812.          0.      19652.     101459.
  ROTOLUENE
    STD.DEV.      31373.        956.       5257.          0.       5874.      43460.

GLYCEROL-1-N          0.          0.        267.          0.          0.        267.
  ITRATE
    STD.DEV.          0.          0.        116.          0.          0.        116.

GLYCEROL-1,2          0.          0.         43.          0.          0.         43.
  -DINITRATE
    STD.DEV.          0.          0.         46.          0.          0.         46.

GLYCEROL-1,3          0.          0.        198.          0.          0.        198.
  -DINITRATE
    STD.DEV.          0.          0.         40.          0.          0.         40.

2-AMINO-4,6-       2054.         39.        271.          0.        430.       2795.
  DINITROTOLUE
  NE
    STD.DEV.       1593.         38.        249.          0.        316.       2196.

GLYCEROL-2-N          0.          0.         29.          0.          0.         29.
  ITRATE
    STD.DEV.          0.          0.         39.          0.          0.         39.

2,4-DINITROT     590057.       1138.      49472.          0.     139758.     780425.
  OLUENE
    STD.DEV.     832363.       1606.      69822.          0.     196793.    1100584.

2,6-DINITROT       6801.        203.        770.          0.       1890.       9664.
  OLUENE
    STD.DEV.       5837.        236.        686.          0.       1720.       8479.

4-AMINO-2,6-       1638.         28.         99.          0.        298.       2064.
  DINITROTOLUE
  NE
    STD.DEV.       2086.         36.        117.          0.        310.       2548.

ALL CHEMS        750061.       2554.      59422.     765127.     162028.    1739193.
    STD.DEV.     920445.       2872.      76289.     944358.     205012.     260259.
```

TABLE A.8-7 SAMPLE OUTPUT OF ALLOCATION MODEL SUMMARY

```
 RATIOS OF REDUCTION IN UNCERTAINTY OVER PROG.COST

AFTER MONTE CARLO SAMPLE    3

.PROGRAM    VAR    CHE  LOC  MED  POP  PCP  EFF    --------PRIOR--------  ------SUBSEQUENT------   DELTA     PROG.COST  RATIO
-------     ---    ---  ---  ---  TYP  IND  ---        HAZARD      SIGMA      HAZARD      SIGMA    SIGMA     DOLLARS   -------

  1 EPI     S      NG        H2O            C          84.57     128.92       72.46      90.91      38.     200000.      .000
  2 EPI     S      NG        H2O            CTG  NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
  3 EPI     S      NG        H2O            CTR  NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
  4 EPI     S      HMX       H2O            C         251.48     426.13      170.82     278.91     147.    200000.      .001
  5 EPI     S      HMX       H2O            CTG  NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
  6 EPI     S      HMX       H2O            CTR  NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
  7 EPI     S      RDX       H2O            C         642.72     570.20      571.13     583.18      0.*   200000.     0.000
  8 EPI     S      RDX       H2O            CTG  NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
  9 EPI     S      RDX       H2O            CTR  NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
 10 EPI     S      HEX       H2O            C            .01        .01         .01        .01      0.     200000.      .000
 11 EPI     S      HEX       H2O            CTG  NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
 12 EPI     S      HEX       H2O            CTR  NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
 37 MUT     S      HMX       H2O            C         251.48     426.13      312.14     533.77      0.*     1100.     0.000
 38 MUT     S      RDX       H2O            C         642.72     570.20      629.59     568.76      1.      1100.      .001
 39 MUT     S      CHX       H2O            C       50213.41   54666.89    45780.98   45494.46    9172.     1100.     8.339
 40 MUT     S      HEX       H2O            C            .01        .01         .01        .01      0.*     1100.     0.000
 41 MUT     S      SEX       H2O            C            .50        .79         .77       1.29      0.*     1100.     0.000
 42 MUT     S      NGU       H2O            C         222.60     375.23      106.54     171.80     203.      1100.      .185
 43 MUT     S      NDP       H2O            C    NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
110 ECH     LMD    NG        H2O                       84.57     128.92       84.28     132.26      0.*    60000.     0.000
111 ECH     LMD    13D       H2O                      132.27     117.99      131.26     116.65      1.     60000.      .000
112 ECH     LMD    12D       H2O                       28.77      41.16       28.64      39.62      2.     60000.      .000
113 ECH     LMD    1MG       H2O                      178.13     174.72      177.40     174.27      0.     60000.      .000
114 ECH     LMD    2MG       H2O                       19.24      32.08       19.24      32.08      0.     60000.     0.000
115 ECH     LMD    TNT       H2O                    67639.04   66148.92    54443.28   51183.06   14966.    60000.      .249
116 ECH     LMD    26D       H2O                     6442.55    8189.85     6442.55    8189.85      0.     60000.     0.000
117 ECH     LMD    24D       H2O                   520283.22  899257.26   512021.72  884724.35   14533.    60000.      .242
118 ECH     LMD    4AD       H2O                     1375.77    2160.12     1375.77    2160.12      0.     60000.     0.000
119 ECH     LMD    2AD       H2O                     1863.01    2239.23     1863.01    2239.23      0.     60000.     0.000
120 ECH     LMD    HMX       H2O                      251.48     426.13      189.34     320.03     106.     60000.      .002
121 ECH     LMD    CHX       H2O                    50213.41   54666.89    50425.43   54957.76      0.*    60000.     0.000
122 ECH     LMD    HEX       H2O                         .01        .01         .01        .01      0.     60000.     0.000
123 ECH     LMD    SEX       H2O                         .50        .79         .50        .79      0.     60000.      .000
124 ECH     LMD    NGU       H2O                      222.60     375.23      221.98     374.08      1.     60000.      .000
125 ECH     LMD    NDP       H2O               NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
126 ECH     LMD    WPH       H2O               NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
142 TRT     R      NG             HUM                  84.57     128.92       83.43     128.21      1.     15000.      .000
143 TRT     R      13D            HUM                 132.27     117.99      129.40     118.41      0.*    15000.     0.000
144 TRT     R      12D            HUM                  28.77      41.16       27.66      39.96      1.     15000.      .000
145 TRT     R      1MG            HUM                 178.13     174.72      178.13     174.72      0.     15000.     0.000
146 TRT     R      2MG            HUM                  19.24      32.08       19.24      32.08      0.     15000.     0.000
147 TRT     R      TNT            HUM              NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
148 TRT     R      26D            HUM                6442.55    8189.85     4663.74    6188.93    2001.     15000.      .133
149 TRT     R      24D            HUM              520283.22  899257.26   446671.73  772048.92  127208.    15000.     8.481
150 TRT     R      4AD            HUM                1375.77    2160.12     1931.83    3113.54      0.*    15000.     0.000
151 TRT     R      2AD            HUM                1863.01    2239.23     2168.21    2686.34      0.*    15000.     0.000
152 TRT     R      HMX            HUM                 251.48     426.13      260.67     441.79      0.*    15000.     0.000
153 TRT     R      RDX            HUM                 642.72     570.20      646.84     574.06      0.*    15000.     0.000
154 TRT     R      CHX            HUM               50213.41   54666.89    74564.58   91520.27      0.*    15000.     0.000
176 SSM     Q      NGU  RAD  H2O                      222.60     375.23      238.93     401.25      0.*    15000.     0.000
177 SSM     Q      HEX  HOL  H2O                         .01        .01         .01        .01      0.     15000.      .000
178 SSM     Q      SEX  HOL  H2O                         .50        .79         .49        .77      0.     15000.      .000
179 SSM     Q      TNR  LCY  H2O               NO VALUE FOR THIS PROGRAMS VARIABLE IN DATA BASE
189 SSM     Q      LWO  RMA  GWT                      198.58     324.30      910.51    1468.89      0.*    20000.     0.000
190 SSM     Q      MPA  RMA  GWT                       35.14      31.49       39.15      34.99      0.*    20000.     0.000
191 SSM     Q      IMP  RMA  GWT                        4.02       6.48         .93       1.48      5.     20000.      .000
192 SSM     Q      CHL  RMA  GWT                    93067.58   93437.79    29558.94   25501.74   67836.    20000.     3.392
 *  INDICATES A REMOVED NEGATIVE DELTA SIGMA.
```

is smaller than the prior if the pattern of random numbers is "unlucky." Furthermore, increasing the number of Monte Carlo samples does not improve this behavior as quickly as one might suppose. Part of the difficulty is due to the fact that the model currently computes mean and standard deviation in the aggregate hazard on a simple arithmetic basis. Because the distribution is skewed toward higher values of hazard, there is a strong possibility that these values will unduly affect the statistics calculated by the Monte Carlo simulation. Accordingly, a variation in which a geometric basis is used (mean and standard deviations of the logarithms of the hazards are computed) is currently under test.

A.8.2.3 Ranking and Evaluation of Studies

As the computer implementation process is still under development, no definitive discussion of the allocation methodology results is yet possible. However, some guidance is possible on how to interpret and use the results.

Programs showing ratios between .001 and .999 are candidates for selection, but may be weak ones. The benefit-to-cost ratios are not high enough to make them especially attractive. However, these ratios should not be interpreted as indicating necessarily that the program is worth less than what it costs. Decisions should be made on a case-by-case basis.

Ratios in excess of 1.000 are likely to be attractive candidates, subject to confirmation by examination of the input assumptions. Thus, in Table A.8-7, mutagenic testing on cyclohexanone, treatment efficacy of 2,4-dinitrotoluene, and source strength monitoring on thiodiglycol seem to be attractive programs. The mutagenic assay shows up primarily through its low costs, whereas the other two combine moderate costs with moderate effectiveness.

A.8.2.4 Conclusions and Recommendations

At present, conclusions about the allocation methodology are limited to the following:

(1) The design of the methodology constitutes a consistent and logical approach to the assignment of research priorities.

(2) The computer implementation of the methodology is partially operational, but needs improvement before it can be used with confidence for all program selections.

(3) Preliminary applications of the methodology suggest that a majority of potential programs may rather low in their benefit/cost ratios, but some programs are clearly quite valuable, either through low cost or through substantial uncertainty reduction potential.

Accordingly, the recommendations emphasize making the methodology fully operational:

(1) The methodology and its computer implementation should be modified to stabilize the Monte Carlo simulation of uncertainties.

(2) Capabilities should be added to the computer model model to evaluate programs with more than one study and studies that reduce the uncertainty in more than one variable.

(3) The computer model should be modified to evaluate the effectiveness of measuring concentrations when none have been measured previously.

(4) Other minor modifications to the computer model should be made to make the outputs more comprehensible and traceable.

Annex A.A

1. LIST OF ABBREVIATIONS

Code	Abbreviation	Reference, if Applicable
7307	Munitions-Related Water Pollutants	Rosenblatt et al., 1973
7409	Munitions-Related Air Pollutants	Mura et al., 1974
7508	Environmental Pollutants at RMA	Rosenblatt et al., 1975a
7509	Physical, Chemical, Toxicological and Biological Properties	Rosenblatt et al., 1975b
ACS	Advances in Chemistry Series	American Chemical Society, 1968
AGCENS	Census of Agriculture	Bureau of the Census, 1972
BDB	Biology Data Book	Altman, 1974
BOD_5	Five Day Biochemical Oxygen Demand	Sawyer, 1971
Browning	Toxicity and Metabolism of Industrial Solvents	Browning
CA	Chemical Abstracts	*
CAMG	Commercial Atlas and Marketing Guide	Rand McNally, 1973
CDM	Climatological Diffusion Model	EPA, 1973
CEH	Chemical Economics Handbook	SRIa
CENSUS	Census of Population, 1970	Bureau of the Census, 1974
CHEMLINE	Chemline	†
COD	Chemical Oxygen Demand	Sawyer, 1971
CTCP	Clinical Toxicology of Commercial Products	Gleason, 1969
DCP	Directory of Chemical Producers	SRI, 1974
Dill	Handbook of Physiology	Dill, 1964
Doyle	G. J. Doyle et al.	Doyle, 1975
EB	Environmental Biology	Altman, 1966
Fairhall	Industrial Toxicology	Fairhall, 1957
HBT	Handbook of Toxicology	Spector, 1956
Hendry	Journal of Physical Chemistry Reference Data	Hendry, 1974
HCP	Handbook of Chemistry and Physics	Weast, 1975

Code	Abbreviation	Reference, if Applicable
H&H	Industrial Toxicology	Hamilton & Hardy, 1974
IARC	International Agency for Research on Cancer Monograph Series	IARC, 1972
Lambert	Sorption in Soil	Lambert, 1967
Lange	Lange's Handbook of Chemistry	Dean, 1973
LC50	Concentration Lethal to 50% of Exposed Population	NIOSH, 1974
LD50	Dose Lethal to 50% of Exposed Population	NIOSH, 1974
LDLO	Lowest Dose Reported as Lethal	NIOSH, 1974
MERCK	Merck Index	Steiber, 1968
NCC	National Climatic Center	†
NIOSH500	National Institute for Occupational Safety and Health List	NIOSH, 1975
NSF	National Science Foundation Study	SRI, 1975
Patty	Industrial Hygiene and Toxicology	Patty, 1963
PHS 149	Survey of Compounds Which Have Been Tested for Carcinogenic Activity	Shubik
Prosser	Comparative Animal Physiology	Prosser, 1973
SA	Statistical Abstract of the United States	Census, 1974
Sax	Dangerous Properties of Industrial Materials	Sax, 1975
TLV	Threshold Limit Value	ACGIH, 1971
TSL	Toxic Substances List	NIOSH, 1974
TVA	Tennessee Valley Authority Files	Private communication
USGS	U.S. Geological Survey Water Data	USGS
WE	The Water Encyclopedia	Todd, 1970
Wilson	Journal of Chemical and Physical Reference Data	Wilson, 1972
WQC	Water Quality Criteria	EPA, 1972
WQCDB	Water Quality Criteria Data Book	Various

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[*] See Abstracting Service in References.

[†] See Computer-Based Data File in References.

Annex A.A

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Abstracting Service

Chemical Abstracts, American Chemical Society (CA)

Computer-Based Data File

National Climatic Center, National Oceanic and Atmospheric Administration, Asheville, N.C.

Annex A.B

PROCEDURES FOR PREPARING INPUT DATA

The main text has given an overview of the hazard estimating and ranking system and the allocation methodology and their implementing computer programs. However, there are many manual operations that may be required to generate the input data for these programs. The programs themselves and the procedures for coding data are described in the following annex. This annex describes, in as few words as possible, the manual operations to be conducted by the system operators, and makes suggestions for estimating procedures, default values, and data sources. Additional details and alternative procedures are described in "Directory of Estimation Procedures of Data Elements and Uncertainties" by Mitchell J. Small. The individuals listed in the Frontispiece and Preface may be consulted for further explanations.

References to source material is given in this section mostly by abbreviations which are listed in the previous annex (A.A) and there indexed to the list of references.

A.B.1 Basic Steps for Preparing Hazard Data

The following general steps will ordinarily be encountered in preparing input data for the hazard model.

A.B.1.1 Review Hazard Algorithm

(1) Determine what hazards (six-subscript level) must be estimated for the problem being addressed.

(2) Review the basic hazard algorithms (Section A.3.1) to specify the variable values needed and the medium (media) that will be affected. Review the appropriate media concentration algorithms (Section A.4-A.6). Determine which variable values (data elements) are already entered in the data base and which must be added or revised.

(3) Check records for subscript codes already in use. Define new ones as required and add to records.

A.B.1.2 Prepare Data Sheet

(1) Select computer report data sheets for each of the data elements that need to be entered.

(2) Review data estimating procedures for each sheet and retrieve necessary background data sources.

(3) Enter codes and subscripts for each data element to be estimated.

(4) Conduct any manual estimating steps required, guided by the following sections.

(5) Review estimates with knowledgeable experts.

(6) Convert estimates to units acceptable to the computer program (Annex A.C).

(7) Enter data and units into data sheets.

(8) Make sure that subscripts have all been defined on Data Sheet I.

(9) Have data punched.

A.B.1.3 Estimate Uncertainty Values

(These steps will ordinarily be conducted simultaneously with those of previous section.)

(1) Use standard uncertainty estimates if the data element satisfies the conditions specified in the procedure.

(2) Otherwise, estimate uncertainty on any basis available (multiple data sources, physical limits, distribution of other estimates, the 20-to-1 bet).

(3) Review the uncertainty estimates with knowledgeable experts.

(4) Code the uncertainty on the data sheets. Be sure to leave column 55 blank for multiplicative (*) or absolute uncertainties (same units as value estimate); use P for percent uncertainties.

A.B.1.4 Document Estimates

(1) The operator should document all estimates for later verification.

(2) Any manual work sheets should be kept in a dated binder.

(3) Any unusual assumptions should be stated in the work sheets.

(4) Complete the documentation section of the data sheets by entering

  (a) Standard source (abbreviations from Annex A.A).

  (b) "Hard" source (enter brief title and date, and so on)

  (c) Name of expert supplying or confirming estimate, or

  (d) Name of operator supplying default value

  (e) Always add date to documentation

  (f) Use continuation column (enter C in 72) whenever needed.

A.B.1.5 Operate Computer System

(1) Divide data base into convenient files of related data (for example, air pollutants). This may require some duplication of data for certain elements, but is well worth it from the standpoint of computer requirements.

(2) Add new or revised data to file. Be sure to remove outdated information.

(3) Check structure of data deck.

(4) Run computer program HERS or AMRDCP (Annex A.C).

A.B.1.6 Review Output

(1) Examine output of computer run, looking for unusual values of aggregate hazard in the summary table.

(2) Trace unexpected zeros to input data. Program will ordinarily indicate when an expected data element has not been entered. Check data cards for inputs to unexpected high or low hazards. Work back through the six-subscript hazards to the input data.

(3) Review outputs with technical experts and revise data if necessary.

(4) Rerun computer program as required.

A.B.2 Source and Dilution Terms

A.B.2.1 Discharge Quantities (Q_{ijm})

If chemical is directly discharged:

(1) Search for Army documents giving discharges (7307, 7409, 7508).

(2) Search for data from which discharges might be estimated: concentration in outfall to water, or in stack gases, or in ponds holding pollutants; rates of wastewater or stack gas discharge. Multiply in correct units.

(3) Search for production information on base material (TNT, NG, HMX/RDX, NGU). Scale discharge quantity to production at another plant. Revise estimate upward or downward if information on relative effectiveness of control measures is available. Search for percentage levels of contamination in another chemical and scale to its discharge rate.

(4) Use default values:

Q_{ij} AIR = 1000 kg/yr

Q_{ij} H_2O = 100 kg/yr

Q_{ij} GWT = 1000 kg/yr

These are also used for a presumed unknown chemical in Program CHI.

(5) Estimate uncertainties:

For (1), as given in sources, or use + 25P

From given uncertainties in (2), or use *2

For estimates from (3), use *3 to *5 depending on quality

For default values, *100.

(6) Enter on data sheet V (Figure A.C-5)

For transformation products:

(1) Determine total rate constant λ_{im} for disappearance of parent, i (A.B.3) from medium m, in yr^{-1}.

(2) Sum input rate for transfers from other media and direct input rate for parent (Q_{ijm}). Call this Q^{s}_{ijm}.

(3) Determine rate constant for transformation into the product i', $\lambda_{ii'}$ (A.B.3).

(4) Calculate transformation product discharge rate as

$$Q_{i'jm} = \frac{\lambda_{ii'}}{\lambda_{im}} Q^{s}_{ijm} \quad .$$

(5) Modify as appropriate with additional information. If process is likely to result in several products, divide $\lambda_{ii'}$ equally among them unless yield ratios are known.

(6) Use uncertainties of $\lambda_{ii'}$, λ_{im}, and Q_{ijm} to help estimate uncertainty in $Q_{i'jm}$, or use *5.

(7) Enter on data sheet V (Figure A.C-5).

A.B.2.2 Concentration Multipliers (c_{ijnk})

(1) Review SRI and EPA versions of Climatological Dispersion Model (Annex A.C.3 and CDM).

(2) Determine coordinates of center of populations-at-risk, (n,k) in m. (See also A.B.4.1.) Suggest no more than 10 of these per location.

(3) Determine coordinates of source(s) (i, j) on same grid. May be defined as (0,0).

(4) Determine values of CDM parameters (see A.C.3 and CDM).

Default values:	Stack diameter 0.5 m
	Stack height 15 m
	Stack temperature 30°C
	Stack velocity 1 m/sec.

(5) Obtain data on wind frequencies for nearest reporting station from NCC, if not already available.

(6) Estimate pollutant half-life, in sec, from A.B.3.

(7) Prepare input data cards.

(8) Run the CDM model.

(9) Retrieve "concentration all sources" from CDM output. Divide by number of sources if more than one is used. Units are UG SEC/GM MT3.

(10) <u>Or</u> use concentration multipliers for a similar chemical at the same location.

(11) Or use concentration multipliers for a similar chemical at a nearby location, interpolating to new population group coordinates on a map.

(12) Estimate uncertainties

For step (9), use *2

For step (10), use *3

For step (11), use *5.

(13) Enter on Data Sheet VI (Figure A.C-6).

A.B.2.3 River Volume Flows (f_{jnk})

(1) Obtain the volume flows (volume per unit time) moving past specified population groups (nk) for annual average and low flow conditions.

(2) Determine the downstream distances from source j to the populations, from USGS or by map measurement (see also A.B.4.1).

(3) Determine the average flow and 7Q10 values for several gaging stations along the downstream portions of rivers affected, from "Water Resources Data" yearbooks.

(4) Interpolate or extrapolate levels to the population groups. Take confluences into account if likely to be of major influence.

(5) Or determine annual discharges of rivers at their mouths from WE and reduce them by any known confluences. Extrapolate or interpolate as necessary.

(5) Or estimate river width from maps, estimate river depth or use 10 m, and calculate cross-sectional area at the population group. Multiply by river velocity or use 0.3 m/sec to get flow.

(7) Use low flows as 0.15 times annual averages if no other information is available.

(8) Estimate uncertainties

For (4), use stated uncertainties or + 20P for average and *3 for low.

For (5), use + 30P for average and *4 for low.

For (6), use *3 for average and *5 for low.

(9) Enter on Data Sheet VII-A (Figure A.C-7).

A.B.2.4 Groundwater Parameters

(1) Review Section A.6.

(2) Obtain maps of groundwater base data if available: bedrock and water table, altitude, aquifer saturated thickness, and transmissivity.

(3) Draw a grid (for example, 1 km) on the downstream aquifer.

(4) Calculate the velocity at each grid point from the equation in Section A.6.4.2.

(5) Determine the location of likely groundwater injection for a chemical.

(6) Sketch the path of maximum velocity from this point and the lines of constant bedrock altitude from points along it.

(7) Locate wells serving populations (n,k) in the downstream field.

(8) Calculate the average velocity, v_{ij}, in cm/sec, to the well(s) of most interest by integrating along the path to their vicinity.

(9) Determine z_{ij}, x_{ij}, and s_{ij} (in km) to each well by measuring along the path and along the bedrock isopleths.

(10) If sample concentration data exist, determine the coordinates of the sample wells similarly, and plot the data as shown in Figure A.6-4.

(11) Determine the data elements Q_{ijm} and D_{ij} from an eyeball (or calculated) regression line.

(12) <u>Or</u> use $D_{ij} = 18$ cm^2/sec as default.

(13) Gather information on discharges to the source reservoir from 7508 and similar Army sources and scale Q_{ijm} to known pairs of discharge/source strength estimates. Use $Q_{ijm} = 1000$ kg/yr as default.

(14) Using base data maps, determine several stretches along a river that carries off the groundwater. These are identified by n = GWO (groundwater outfall) and by k.

(15) Determine the lengths of these stretches, L_{jnk}, the local values for the gradient, g_{jnk}, and the transmissivity, TR_{jnk}.

(16) Determine a typical porosity, P_j, for the general location, using Table 4-25 of WE.

(17) Estimate uncertainties--see Table A.B-1.

(18) Enter on Data Sheets VIII-A, VIII-B, and VIII-C (Figures A.C-10 through 12).

Table A.B-1

DEFAULT UNCERTAINTIES
FOR GROUNDWATER PARAMETERS

Parameter	If (11) is Used	If (12) is Used
z_{ij}, s_{ij}	+ 10P	+ 10P
v_{ij}	* 2	* 2
D_{ij}	+ 10P	+ 30P
Q_{ijm}	* 2	* 5
Q default	--	* 100
g_{jnk}	+ 10P	+ 10P
TR_{jnk}	+ 10P	+ 10P
L_{jnk}	+ 10P	+10P
P_j*	* 1	* 1

---

*Porosity is programmed into the model at 0.4. If another location is considered, P may be changed, but is considered to be known exactly.

A.B.2.5 Direct Concentration Inputs (C_{ijmnk})

(1) Concentration data may be available directly for specified population groups, either from measured data or from the output of a subsidiary model. The CDM is essentially a subsidiary model in this sense.

(2) The output of a sampling program or a subsidiary model should be expressed in the usual concentration units--UG/MT3 for AIR and MG/LT for H2O and GWT.

(3) Concentrations may be interpolated to the coordinates of population groups if required.

(4) Estimate uncertainties

For measured AIR Concentrations: *2

For measured H2O concentrations: *2

For measured GWT concentrations: *3

For modeled concentrations: infer from discusssion of model or use *5.

(5) Enter on Data Sheet IX (Figure A.C-13).

(6) Typical ranges for concentrations are

AIR: 0.01 - 5.0 UG/MT3

H2O: 0.000001 - 1.0 MG/LT

GWT: 0.0001 - 0.01 MG/LT.

A.B.3 Environmental Chemistry

A.B.3.1 Physical Transfers

(1) The purpose of these procedures is to estimate the contribution of physical processes to the disappearance of a chemical from a medium, in terms of a first-order rate constant λ_{im}. A subsidiary purpose, not fully implemented, is to estimate inputs to a medium from other media, for example, inputs from land to groundwater to surface water.

(2) The processes considered are volatilization from soil or water to air (soil loss rate assumed equal to water loss rate); deposition from water onto sediments; deposition from air onto soil; transfer from soil (waste basins) to groundwater; and transfer from groundwater to surface water. The last was treated in A.B.2.4.

(3) Obtain molecular weight, M, vapor pressure, VP (mmHg = Torr at 20-25°C), and solubility SB (mg/ℓ at 15-20°C) from Army documents, HCP, Merck, Lange, Timmermans (1965), Jordan (1954), and so on.

(4) If solubility is not available explicitly, use the following values for qualitative descriptions:

Miscible:	5×10^6 mg/ℓ
Very soluble:	5×10^5 mg/ℓ
Soluble:	5×10^4 mg/ℓ
Slightly soluble:	10^3 mg/ℓ
Insoluble:	10^2 mg/ℓ
No data:	10^3 mg/ℓ

(5) If vapor pressure is given at other than 20-25° C, multiply by following factors:

0°	3.0	60°	0.1
10°	1.5	70°	0.07
30°	0.7	80°	0.03
40°	0.3	90°	0.02
50°	0.2	100°	0.01

(6) In HCP, 51st edition, p. D146 ff, vapor pressure can be derived by using A and B in the equation

$$VB = 10^{(B-.0007457A)}$$

(7) If no VP information, use 0.01 mmHg.

(8) Estimate rate constant for volatility by expression derived from MacKay and Wolkoff (1973):

$$\lambda_V = 230 \frac{VP \times M}{SB} \text{ yr}^{-1}$$

(9) Check with qualitative descriptions

Highly volatile	$\lambda_V > 100$
Moderately volatile	$100 \geq \lambda_V > 10$
Slightly volatile	$10 \geq \lambda_V > 1$
Not volatile	$1 \geq \lambda_V$

(10) Estimate rate constant for deposition from water or groundwater by the SRI-derived approximation*

$$\lambda_{DW} = 7{,}000/SB \text{ yr}^{-1}$$

(11) Estimate rate constant for deposition from air by

$$\begin{aligned} \lambda_{DA} &= 2.0 \text{ yr}^{-1} && VP < 0.01 \\ &= 0.7 \text{ yr}^{-1} && 0.01 \leq VP < 1.0 \\ &= 0.07 \text{ yr}^{-1} && 1.0 \leq VP < 100 \\ &= 0.0 \text{ yr}^{-1} && 100 \leq VP \end{aligned}$$

---

*If a more accurate treatment is desired, refer to Lambert (1967).

(12) Estimate rate constant for percolation from basins to groundwater by the SRI-derived approximation

$$\lambda_P = 0.01 \text{ SB/M yr}^{-1}$$

(13) Estimate uncertainties:

In VP and S:
If measured used *2
If from table use *3
If default use *10

In λ's:
If contain only VP or SB, use uncertainty of that.
If contains both, use

$$\ell n\, U_\lambda = \sqrt{\left(\ell n U_{VP}\right)^2 = \left(\ell n U_{SB}\right)^2}$$

(14) Enter in worksheet (Table A.B.2).

A.B.3.2 Chemical Transformations

(1) The purpose of these procedures is to estimate the contribution of chemical and biochemical processes to λ_{im}. A subsidiary purpose, not fully implemented, is to estimate inputs to the same medium of transformation products of the original chemical.

(2) The processes considered are hydrolysis (attack by OH^-), oxidation (attack by oxidants), photolysis (attack by electromagnetic radiation), photooxidation (combined action of last two), and biodegradation (attack by microbes).

(3) The applicability of the various processes in different media is shown in Figure A.3.3.

(4) Search literature for information on rate constants, at known reactant concentrations: Hendry, Wilson, ACS, Doyle, or CA.

Table A.B.2

RATE CONSTANT WORKSHEET
(in yr^{-1})

λ_{DA} = ________	U = ________	λ_{DW} = ________	U = ________	λ_{DW} = ________	U = ________
		λ_{V} = ________	U = ________	λ_{P} = ________	U = ________
λ_{OA} = ________	U = ________	λ_{OW} = ________	U = ________	λ_{OW} = ________	U = ________
λ_{PH} = ________	U = ________	λ_{PH} = ________	U = ________		
		λ_{H} = ________	U = ________	λ_{H} = ________	U = ________
		λ_{B} = ________	U = ________		
λ_{AIR} = ________	U = ________	λ_{H2O} = ________	U = ________	λ_{GWT} = ________	U = ________

(5) Assume the following reactant concentrations:

$[O_3]$ in air: 2×10^{-9} M
$[\cdot OH]$ in air: 10^{-15} M
$[RO_2\cdot]$ in water: 10^{-10} M
Solar flux: 2.2×10^{-7} einsteins/cm^{2}sec
Quantum yield: 10^{-2}
pH: 7

(6) Estimate the rate constant for hydrolysis from the pseudo-first order constant k_H (sec^{-1}):

$$\lambda_H = 3.15 \times 10^7 \, k_H \qquad \mathrm{yr}^{-1}$$

(7) Estimate the rate constant for oxidation in water from the bimolecular rate constant, K_{RO_2} (M^{-1} sec^{-1}) by

$$\lambda_{OW} = 3.15 \times 10^7 \, K_{RO_2} \, [RO_2\cdot] \qquad \mathrm{yr}^{-1}$$

(8) Estimate the rate constant for oxidation in air from the bimolecular rate constant for ozone, K_{O3} and hydroxyl radical, k_{OH}, as

$$\lambda_{OA} = 3.15 \times 10^7 \left(k_{.OH}[\cdot OH] + K_{O3}\,[O_3]\right) \qquad \mathrm{yr}^{-1}$$

(9) Estimate the rate constant for photolysis, λ_{PH}, only for those compounds that are known or assumed to be photoactive (Wolfe, 1976).

(10) Estimate the rate constant for biodegradation from the BOD and COD, if known:

$$\lambda_B = 69.3 \, \ell n \, \frac{COD}{COD - BOD_5} \qquad \mathrm{yr}^{-1}$$

where COD is expressed in mg/ℓ oxygen per mg/ℓ chemical concentration, and BOD_5 is expressed in the same units (in the limit as concentration goes to zero). Otherwise use qualitative information if no actual rates are reported (assume first-order kinetics even though unlikely in practice):

Easily biodegradable:* $\lambda_B = 100\ \text{yr}^{-1}$

Moderately biodegradable: $\lambda_B = 10\ \text{yr}^{-1}$

Sparingly biodegradable: $\lambda_B = 1\ \text{yr}^{-1}$

(11) When no definite information on rate constants is found, argue from chemical similarity.

(12) If hydrolysis constant is available at another pH, adjust by dividing by 10^{α} where α is the absolute value of pH - 7.

(13) For both hydrolysis and oxidation, if data is available at a higher temperature, adjust by dividing by 2^{β}, where $\beta = (T-20)/10$, with T in °C.

(14) Or use default values

$\lambda_H = 0.1\ \text{yr}^{-1}$

$\lambda_{OW} = 0.3\ \text{yr}^{-1}$

$\lambda_{OA} = 0.3\ \text{yr}^{-1}$

$\lambda_{PH} = 1.0\ \text{yr}^{-1}$

$\lambda_B = 0.1\ \text{yr}^{-1}$

(15) Use same values for groundwater hydrolysis as for surface water.

(16) Estimate uncertainties:

From descriptions in literature

For well-documented estimates, use *2

For partially-documented estimates, use *10

For default values, use *200.

(17) Enter in Worksheet (Table A.B-2).

A.B.3.3 Net Rate Constants

(1) Calculate $\lambda_{AIR} = \lambda_{PA} + \lambda_{OA} + \lambda_{PH}$

(2) Calculate $\lambda_{H2O} = \lambda_{DW} + \lambda_V + \lambda_{OW} + \lambda_{PH} + \lambda_H + \lambda_B$

(3) Calculate $\lambda_{GWT} = \lambda_{DW} + \lambda_{OW} + \lambda_H$

---

*A BOD_s indicative of 70% satisfaction corresponds to a λ_B of about 80.

(4) Estimate uncertainty

If one is dominant, use its uncertainty.

Otherwise, use

$$U_{\lambda} = \lambda \sqrt{\sum_{t} \left(\frac{U_{\lambda t}}{\lambda_{t}} \right)^{2}}$$

where the λ_t are the contributing rate constants.

(5) Enter λ_{H2O}, U_{H2O} in Data Sheet VII-B.

(6) Use λ_{AIR} in CDM, if appropriate

A.B.3.4 Transit Times (t_{jnk})

(1) Value desired is time (in yr) required for an average molecule of chemical to move from point of discharge (j) to group k of population n. Applies only to river water at this time.

(2) Data are sometimes directly available from studies of rivers (for example, those done by the TVA) or for gage stations in river sections of interest (see A.B.2.3). Forms 9-275 can be obtained from USGS for these stations, from which velocity-flow relations can be derived.

(3) Otherwise, determine downstream distance (km) to group k from USGS maps and divide by 10^4 km/yr for ordinary streams or by 1.5×10^4 km/yr for steeper ones.

(4) Estimate uncertainties

for (2): + 20P
for (3): * 1.5

(5) Enter in Data Sheet VII-A (Figure A.C-7).

A.B.4 Exposures

A.B.4.1 Populations-at-Risk (N_{jmnk})

(1) Define the location, j, of pollutant discharge of concern.

(2) Acquire USGS maps of the area surrounding the location; scales of 1:250,000, 1:62,500, and 1:24,000 may be useful.

(3) Locate discharge point(s) on map.

(4) For air pollutants, examine wind frequency data (see Annex A.C.3.1) for any prevailing winds, and sketch a rough ellipse with focus on discharge point, long axis of ~30 km along prevailing wind, and eccentricity roughly related to degree of prevalence. Alternatively, make a 4 km × 4 km grid and run nodes through SRICDM. Draw rough contours, then select as "area of concern" the region in which SMC ≥ 0.02 $(\mu g/m^3)/(g/sec)$.

(5) For water pollutants, identify rivers downstream of discharge point, major confluences, and so on.

(6) For groundwater pollutants, identify aquifer flow field downstream of discharge point (see A.B.2.4) and river(s) carrying off groundwater and sketch a map.

(7) Identify any centers of human population in or near the areas identified in (4)-(6) above.

(8) For air pollutants, choose about 5-10 of the largest towns in the area as the population groups k. If a large city has areas significantly different in distance or direction from the discharge, subdivide it. (Maps of census tracts for this purpose are available in CENSUS.)

(9) For water pollutants, choose about five of the largest towns downstream within about 300 km that use river water for drinking. (These are sometimes listed in Problem Definition studies. Cities that use river water may otherwise be identified by contacts with state or local officials, such as the City Water Commissioner.)

(10) For groundwater pollutants, choose about five of the largest population centers within about 20 km in the downstream field. If possible, identify whether groundwater is used, and the location of the well(s) from local contacts. Otherwise, assume it is used, and choose a likely well from the USGS quad map.

(11) Determine populations (N_{jmnk}) associated with these centers. Any reasonable source is probably accurate enough. CAMG is usually sufficient, but CENSUS may be necessary for subdividing cities. For unincorporated areas, buildings shown on USGS may be counted and multiplied by four to estimate population (check date of map). Sometimes data are available from special studies, like those on water supply.

(12) For air pollutants, identify counties with significant areas in rough ellipse.

(13) Determine crop acreage (total) and crop acreage (hay) from Table 8 in AGCENS, subtract hay acreage from total acreage to obtain N_{jmnk} for crops.

(14) Choose a point within county to represent location of crops.

(15) If county is spread out, can subdivide into areas on basis of USGS maps, and apportion total acreage accordingly.

(16) For water pollutants, identify impoundments (lakes, reservoirs, wide parts of the river) where high populations of fish might occur.

(17) Estimate number of "\$1" fish in lakes from fish counts (state Departments of Fish and Game seldom helpful) or from area[*] of lake (0.05 \$1 fish/m^2).

(18) No other populations are currently estimated. However, livestock populations are available on a county basis from AGCENS, Table 7.

(19) Alternative choices may be made if the problem appears to be concentrated in one region after the model is run.

---

[*] Most productivity near surface; for streams a volume factor of 0.005 \$1 fish/m^3 may be better.

(20) Estimate uncertinty:

For (11): Usually use +20P
If subdivided, use +30P
If map used, use *2.

For (13): Use +30P
If subdivided, use *2.

For (17): Use *2
If estimated from area of volume, use *5.

(21) Enter in Data Sheet II (Figure A.C-2).

A.B.4.2 Dose-to-Concentration Ratios ($b_{im\ell}$)

(1) Determine from toxicological indications whether effect ℓ is dependent on concentration or total dose (see A.B.5).

(2) Use 500 liter/yr for water ingestion, 7,300 m^3/yr for air inhalation, for humans.

(3) All fish and crop effects are currently assumed to be concentration dependent.

(4) Selected other annual exposure factors ($b_{im\ell}$) are given in Table A.B.3.

(5) Estimate uncertainty as *1.6 for humans to account for variations in personal habits, size, and so on.

(6) Enter in Data Sheet IV (Figure A.C-4).

A.B.4.3 Water Treatment Efficacy (R_{in})

(1) Search pollution control literature for treatment data on specific compound. (Rarely successful.)

(2) Or relate chemical structurally to one in Table A.5-3 and use similar factor.

(3) Or use default value of 0.3.

Table A.B-3

EXPOSURE FACTORS[*]

Species	Weight (kg)	Food Intake (kg/yr)	Water Intake[†] (l/yr)	Air Intake[‡] (m^3/yr)
Man	65	550	450	7,000
Monkey	5	90	--	850
Dog	10	275	350	2,000
Cat	2	37	--	800
Cattle	500	2,750	17,000	60,000
Horse	500	3,650	8,000	35,000
Sheep	60	875	1,000	8,000
Rabbit	2	22	125	450
Rat	0.4	7	12	280
Mouse	0.02	1	2.5	35
Chicken	2	90	--	600

---

[*] *Use these values with caution*, they are subject to many caveats. Although they are adequate for the purpose of this study, they should not be used for more demanding tasks, such as the development of criteria for standards.

[†] Drinking, doesn't include water in food or water of metabolism.

[‡] Tidal volume--not all is taken in by far (about 8% of the oxygen in the tidal volume is).

Sources: BDB, EB, Prosser

(4) Estimate uncertainty:

For (1)--as suggested by source

For (2)--$*1/R_{in}$ unless $R_{in} < 0.2$, then use *5

For (3)--use *3.

(5) Enter in Data Sheet VII-C (Figure A.C-9).

A.B.5 Effects

A.B.5.1 Human Health Effects

(1) Attempt to enter data for cancer (C), severe chronic effects (CTG), and recoverable chronic effects (CTR) for every chemical. Enter acute toxicity (ATX) only when either acute effects are being observed in the real environment or the chemical is newly being discharged, and no history of safety is available. Define any additional effects on an ad hoc basis.

(2) Purpose is to determine whether effect is concentration-dependent or dose-dependent (defines $b_{im\ell}$) and to estimate the slope of a zero-threshold dose-response relationship ($S_{im\ell}$).

(3) Acquire any applicable toxicologic information: Army reports (e.g., 7509), TSL, WQCDB, Patty, H&H, Fairhall, Merck, CTCP, Sax, HBT. Use data for most sensitive indicator species.

(4) If effect is dose-dependent and measured in animals, the dose may be expressed in mg/kg body weight. Use 60 kg for humans. Assume dose is delivered over a year.

(5) If total dose to animal is given, one can extrapolate on basis of weight, as above, or on basis of surface area (weight to the 2/3 power). In either case, typical animal weights are given in Table A.B.3.

(6) Concentrations affecting animals are assumed to affect humans equally (mg/ℓ water, mg/m^3 air).

(7) Label axes of dose-response plot (Figure A.3-2) with proper dose units on abscissa and fraction affected on ordinate.

(8) Plot any available data on chart: LD50, LC50, LD100, LD10, TVL, and so on.

(9) Eyeball a straight line best fitting the plotted points. At this juncture, a nonzero indicated threshold is acceptable.

(10) Determine the dose, D5, at which a 5% response is predicted.

(11) Estimate $S_{im\ell} = 0.05/D5$.

(12) If only one point (such as, LD50) is available, estimate $S_{im\ell} = 0.5/LD50$, or similarly for other points. However, if a nonzero "threshold" is expected, use $S_{im\ell} = 0.09/LD50$.*

(13) If no data are available, use default values as described below.

(14) If effect is cancer, determine which node(s) of Dehn & Helmes' (1974) activity tree contain the molecular structure of the chemical.

(15) If no likely node is found, use node 3947.

(16) Retrieve p(C) and P for each node for the appropriate route of exposure (inhalation for AIR, oral for H2O or GWT).

(17) Choose the highest product of p(C) and P and compute

$$S_{im\ell} = 0.0005\ p(C)P \quad .$$

(18) If listed in PHS 149, modify as follows:

If results "negative," drop $S_{im\ell}$ to 5×10^{-4}, if originally higher.

If results "positive," increase p(C) to 1.0 and recompute.

If both, no change.

(19) If listed in IARC, increase p(C) to 1.0 and recompute.

(20) If listed in NIOSH 500, increase p(C) to 0.5 (if lower) and recompute.

(21) Use uncertainties shown in Dehn & Helmes (1974) for C--combine by

$$\ln U_S = \sqrt{\left(\ln U_P\right)^2 + \left(\ln U_P\right)^2}$$

---

*This combines two assumptions: (1) the "threshold" is one-half the LD50, and (2) the resulting D5 is used to determine the slope.

(22) Default values for other effects are

CTR - 0.01 /GM

CTG - 0.001 /GM

(23) Estimate uncertainties:

Use any clues suggested by literature or select from Table A.B.4.

(24) Enter in Data Sheet IV (Figure A.C-4).

Table A.B.4

UNCERTAINTIES FOR $S_{im\ell}$

Effect	Data Available from Program	Uncertainty
CTG	90D	*10
	ATM	*33
	Default	*300
CTR	90D (CTR)	*33
	90D (CTG)	*75
	ATM (CTR)	*100
	ATM (CTG)	*200
	Default	*300
ATX	ATM	*10
	Partial data	*33
	Default	*100
FKL	AAT	*5
	SAT	*10
	Default	*100
CFS	CAT	*2
	AAT	*3
	SAT	*25
	Default	*250

A.B.5.2 Other Effects

(1) Attempt to enter data for fish kill (FKL) and chronic fish toxicity (CFS) for every chemical, unless there are data indicating these effects are not important. Enter data for crop yield loss (CYL) only where data suggest there is an effect, since default values have not been generated. Define any additional effects on an ad hoc basis.

(2) Paragraphs (2), (3), (7), (8), (9), (10), (11), (12), (23,), and (24) from A.B.5.1 also apply to this section.

(3) Use data from other species and extrapolate to the species in question. Use data for most sensitive species if in doubt.

(4) Concentration-dependent effects are assumed to apply equally to all species, unless better information is available.

(5) If no data are available for a given chemical, use default values as described below.

(6) If acute data are available for fish, but chronic data are not, compensate for low flow/average flow differences by using

$$S_{CFS} = 3\ S_{FKL}$$

(7) If no acute data are available, use $S_{CFS} = 0.006$ LT/MG YR, $S_{FKL} = 0.002$ LT/MG YR.

(8) Enter on Data Sheet IV.

A.B.6 Valuations ($V_{n\ell}$)

(1) Define the effect ℓ under consideration, both by population type affected and characteristics.

(2) Compare effect subjectively with those already valued (Table A.3-6).

(3) Search literature for any economic indicators (especially SA).

(4) Define units of accounting (cases, acres, pounds, board-feet, and so on).

(5) Estimate value, in \$, for the unit specified for N_{jmnk}.

(6) Estimate uncertainty:

On basis of literature
Similarity to other effects
Default *3.

(7) Enter in Data Sheet III (Figure A.C-3).

A.B.7 Basic Steps for Preparing Allocation Data

The following general steps will ordinarily be encountered in preparing input data for the allocation model.

A.B.7.1 Review Allocation Methodology

(1) Review basic concepts of allocation methodology (Section A.7).

(2) Review input and output of previous cycle of allocation.

(3) Check to see that any new scientific information has been interpreted and added to the hazard data base.

A.B.7.2 Candidate Studies

(1) Check to see if research program status matrix is complete and up to date; if not, add and change as necessary.

(2) Select all candidate studies coded "1" in the status matrix, and record the program code and subscripts applicable to each.

(3) Select any studies with codes "5" or "6" that are serious candidates for repeating.

(4) Select any studies coded "2" or "3" that might have become significantly less attractive in light of new information.

(5) Define all of the projects (variables affected) for each study, and determine the subscripts for each (see Table A.7-2 for guidance).

A.B.7.3 Study Costs and Effectiveness

(1) Determine the cost, C_p, associated with each study, using Table A.7-4 as a guide.

(2) Revise C_p using any knowledge of special conditions (explosive hazard, previous work, and so on) that is available.

(3) Determine the subsequent uncertainties for each of the variables affected by projects in the study, U_X', using Table A.7-2 as a guide.

(4) Revise these uncertainties using any knowledge available (difficulty of performing the experiment, prior information available, and so on).

(5) Check to see that these subsequent uncertainties are smaller than the ones currently in the data base for the same variables. (The computer program will tell you this, but it may be cheaper to look first.) Revise prior or subsequent uncertainties or drop study from consideration.

A.B.7.4 Prepare Data Sheet

(1) Use the AMRDC Priorities Data Sheet (Figure A.C-19).

(2) Prepare a line for each project of each study.

(3) Enter codes PRO for program, the program code (Table A.7-2), code for the variable affected, and all appropriate subscripts.

(4) If the subscript does not apply to the variable in question (for example, subscript n does not need to be specified for $S_{im\ell}$), then leave the subscript blank.

(5) If the subscript does apply, but the project reduces the uncertainty for all variables with subscripts of that type, use XXX as subscript. Example: Sampling (SAM) reduces uncertainties on the concentration of all population groups k at the sampled location j. The entry would read, for example,

AD-A050 782 STANFORD RESEARCH INST MENLO PARK CALIF F/G 5/1
SETTING PRIORITIES FOR ENVIRONMENTAL R AND D ON ARMY CHEMICALS.(U)
JAN 77 S L BROWN DAMD17-75-C-5071
UNCLASSIFIED SRI-CRESS-13 NL

3 OF 3
AD
A050 782

END
DATE
FILMED
4-78
DDC

PRO SAM Cbb MNT VOL AIR HUM XXX bbb (b = blank)

where the variables affected are C_{ijmnk} for all k; ℓ does not apply.

(6) Enter the study cost, variable subsequent uncertainties, and program title (currently limited to 10 characters).

(7) Document inputs on the data sheet and elsewhere, as necessary, as described in A.B.1.4.

(8) Have data punched.

A.B.7.5 Operate Computer System

(1) Divide program cards into sets that operate on a file of related hazard data. For example, all cards showing chemical subscripts of MN, NM, MNT, or TNM would operate with the air pollutant file, and would be unnecessary for any other. This division saves computer run time and storage requirements.

(2) Check structure of allocation program data deck and of hazard file on which it is to operate.

(3) Run computer program AMRDCP (Annex A.C).

A.B.7.6 Review Output

(1) Examine output of computer run, looking for unusual values of the effectiveness/cost ratio in the last column of the summary output.

(2) Trace unexpected zeros: if preceded by *, the subsequent standard deviation in the aggregate hazard is larger than the prior one, which can be checked by examining the appropriate variable uncertainties. Occasionally, the Monte Carlo statistics may generate a spurious zero, and the program must be rerun.

(3) Other zeros may occur if no hazard is affected (zeros in both prior and subsequent hazard). This is usually due to missing input hazard data.

(4) Zeros will occur if errors in input format or program logic have occurred.

(5) Unusually high ratios should also be traced to their origins in the data, and the data revised if they are in error.

(6) Review revised output along with technical inputs and revise again if necessary.

(7) Rerun complete program as required.

(8) Repeat for all sets of data.

(9) Rank the nonzero studies by the effectiveness/cost ratio. Show where the studies have a cumulative cost equalling or exceeding the budget being allocated.

Annex A.C

DATA PROCESSING

Chronologically, the implementation of models developed in this study for computer processing has occurred in three stages:

- The SRI version of the EPA Climatological Dispersion Model (EPA, 1973) was developed as a separate preprocessor for analysis of air pollutant concentrations. This program was documented in January 1976. (Bun, 1976a)

- The HERS hazard estimating program was developed to allow repeated estimation of "deterministic" hazard values from "best estimates" of input variables, and to verify earlier manual calculations. This program was documented in August 1976. (Bun, 1976b)

- The AMRDCP resource allocation program was developed to estimate the "stochastic" hazard uncertainty reduction per unit cost for candidate research studies. The estimation is made through a Monte Carlo simulation of the propagation of the uncertainties in the input variables. This program was documented in December 1976. (Bun, 1976c)

Logically, the CDM is only one of a potentially large set of preprocessors to estimate concentrations on other variables of the model. Accordingly, it is discussed last.

All three programs are operational, but all could be substantially improved with modest additional effort.

The following documentation is a condensation of the most important features of the three programs from the user's point of view. Details, such as sample input and output, program listings, and the like, were reported in the three documents listed above (Bun, 1976a,b,c).

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A.C.1 The Hazard Estimating Program

The hazard estimating program (HERS) implements the hazard models discussed in Sections A.3-A.6, using the equations shown in Sections A.3.2.1, A.4.7, A.5.8, and A.6.9.*

A.C.1.1 Program Specifications

Every input variable and hazard output of the model is identified by some combination of the following six subscripts:

i = Chemical (CHE)
j = Location (LOC)
m = Medium (MED)
n = Population type (PTP)
k = Population group (PID)
ℓ = Effect (EFF)

Each subscript can be assigned an arbitrary alphanumeric value of one to three characters. Most subscripts should have mnemonic content. The preassigned subscripts for the media are AIR for air, H2O for surface water, and GWT for groundwater. The suggested subscripts for population types are HUM for humans, FSH for fish, and CPS for crops. A special "population" type, GWO, is defined to identify the locations of the outfalls of groundwater into surface water.

Each variable is also identified by a code of from one to three characters. The variables currently in use are shown in Tables A.C-1 through A.C-4. The values of each variable must be expressed in dimensionally correct units. However, the program will convert the most common units into CGS units for purposes of computation, and then back into convenient units for output presentation. The units reorganized by the program are shown in Table A.C-5.

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*The hazard estimating program has the capability to accept a threshold value for effects, and also truncates the dose-response relationship at an upper limit of 1.0.

Table A.C-1

INPUT VARIABLES:
HAZARD AND DOSE-RESPONSE CALCULATION

Mathematical Notation	Computer Notation	Contents
N_{jmnk}	N (LOC, MED, PTP, PID)	Population size
$V_{n\ell}$	V (PTP, EFF)	Valuation
$S_{im\ell}$	S (CHE, MED, EFF)	Slope of dose-response curve
$B_{im\ell}^{*}$	B (CHE, MED, EFF)	Threshold of dose-response curve
$b_{im\ell}$	SMB (CHE, MED, EFF)	Dose-to-concentration ratios

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[*] Usually assumed to be zero.

Table A.C-2

INPUT VARIABLES:
AIR POLLUTANT MODEL

Mathematical Notation	Computer Notation	Contents
Q_{ijm}	Q (CHE, LOC, MED)	Emission rate
C_{ijnk}	SMC (CHE, LOC, PTP, PID)	Concentration multiplier

Table A.C-3

INPUT VARIABLES:
WATER POLLUTANT MODEL

Mathematical Notation	Computer Notation	Contents
Q_{ijm}	Q (CHE, LOC, MED)	Effluent rate
f_{jnk}	SMF (LOC, PTP, PID)	Stream flow rate
t_{jnk}	SMT (LOC, PTP, PID)	Transit time
λ_{im}	LMD (CHE, MED)	Transformation-transfer rate
R_{in}	R (CHE, PTP)	Treatment efficacy

Table A.C-4

INPUT VARIABLES: GROUNDWATER POLLUTANT MODEL

Mathematical Notation	Computer Notation	Contents
Q_{ijm}	Q (CHE, LOC, MED)	Inflow to groundwater
Z_{jnk}, X_{jnk}	ZX (LOC, PTP, PID)	Down and cross distance to well or outfall
v_{ij}	SMV (CHE, LOC)	Flow rate in aquifer
D_{ij}	D (CHE, LOC)	Diffusion constant
For Groundwater Outfalls		
$(TR)_{jk}$	TR (LOC, OID)	Transmissivity constant
g_{jk}	SMG (LOC, OID)	Local gradient
L_{jk}	L (LOC, OID)	Length of outfall

Table A.C-5

STANDARD CODES FOR UNITS

Code	Unit
GM	Grams
KG	Kilograms
MG	Milligrams
UG	Micrograms
MT	Meters
CM	Centimeters
KM	Kilometers
LT	Liters
SC	Seconds
YR	Years
DY	Days
$$	Dollars
FT	Feet
SM	Square meters
CT	Count (of humans)
$F	Dollar fish

A.C.1.2 Data Inputs

Data to be entered into the program is coded on AMRDC Pollutant Hazard Model Data Sheets. These are of 13 different formats specialized for encoding 13 separate classes of program inputs. The 13 different classes of program inputs are:

I	Effects, population types, locations, and chemicals
II	Populations
III	Valuation of effects
IV	Slope, threshold, and dose-to-concentration ratios
V	Emission/effluent rates
VI	Air pollutant model--concentration multipliers
VII-A	Water pollutant model--flow rates and transit times
VII-B	Water pollutant model--transformation - transfer rates
VII-C	Water pollutant model--purification factors
VIII-A	Groundwater pollutant model--diffusion constants and flow rates
VIII-B	Groundwater pollutant model--locations of wells and groundwater outfalls
VIII-C	Groundwater pollutant model--transmissivity, gradient, and length of groundwater outfalls
IX	Concentrations*

The inputs from the Class I data sheets define values of four of the six types of subscripts (CHE, LOC, PTP, EFF). The inputs from the Class II data sheets define the population identification (PID) subscripts and give population sizes. The sixth subscript type--medium (MED) is predefined. The remaining classes of data sheets are used for entering data in terms of the predefined subscripts and those defined on the Classes I and II data sheets.

The 13 formats are essentially specializations of the single general format shown in Figure A.3-4. The first datum encoded on each line is entered in a three-column field labeled "Variable." This

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*Currently implemented only in the resource allocation (AMRDCP) version.

datum is a one- to three-letter code for the variable about which information is being provided. Following this is a group of six three-column fields labeled "Subscripts" which contain the alphanumeric subscript values associated with the particular data value. The next 11-column field, "Value," contains the value of the variable in some set of units. The value may be coded as an integer, as a decimal number (with decimal point indicated), or in a scientific notation. In the latter case, the exponent is indicated by a + or - sign followed by the power of 10 desired and is coded "right justified" in the field. If the mantissa is coded without an explicit decimal point, no blank column should occur between the mantissa and the + or - sign of the exponent.

The units in which the variable is described are coded in the next group of fields. Units are coded by putting the appropriate abbreviation in the first two columns of a unit field and the positive power (the power "1" may be represented by a blank) in the third column. List all units with positive powers first. Then code a slash "/" in the next one-column field. Then code all the units with negative powers, indicating their powers by positive numbers. For example, μg cm yr^{-2} is represented by

UG CM/YR2

Population units may be any two-character abbreviation but must not duplicate any code already used for units.

Uncertainty codes can be either additive or multiplicative as indicated by a "+" or "*" in column 49. The uncertainty is coded in 50-54 according to the same rules as for coding value (columns 22-32). If column 55 contains a nonblank character, the coded additive uncertainty is interpreted as a percentage of the given value. For example, +50P coded in 49-55 implies symmetric limits of 0.5X to 1.5X, where X is the value of the datum coded in 22-32. Multiplicative uncertainty factors must be 1 or greater. For example * 1.5 implies limits of 0.667X to 1.5X.

The 16-character Description or Documentation field (columns 56-71) is used to describe subscripts and indicate sources for data.

If a nonblank character is coded in column 72, the next card is read and the data for the Description or Documentation field of this following card is used as a continuation of the previous data. Up to three continuations are permitted (yielding a total of four 16-character fields).

Columns 73-80 may be used to insert a "case code" to identify data sets that go together. For example, if the program were to be run with data as of a specific date, that date could be used as a case code. The case code is also entered on a case title card.

The 13 input forms are shown in Figures A.C-1 to A.C-13. After the information has been keypunched, one line to a card, the cards are arranged in the order shown in Figure A.C-14. Order within the blocks is unimportant.

FIGURE A.C-1

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS

I. Effects, Population Types, Locations, and Chemicals

Case Code

73 74 75 76 77 78 79 80

Variable EFF PTP LOC CHE	Subscripts						Value	Units								+ or −	Uncertainty Codes	b or %	Description of Subscript	Continued
	Sub-script																			
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-2

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS

II. Populations

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units								+ or •	Uncertainty Codes	b or %	Location	Continued
N	Loc j	Med m	Pop Type n	Pop Index k			N_{jmnk}													
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-3

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS

III. *Population Types and Valuations of Effects*

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units								Uncertainty Codes			Documentation	Continued
PV	Effect I	Pop Type P_I					V_I		$$	/						+ or •		b or %		
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-4

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS
IV. Slope, Threshhold and Dose to Concentration Ratios

Case Code

73 74 75 76 77 78 79 80

Variable S B SMB	Subscripts						Value	Units								+ or •	Uncertainty Codes	b or %	Documentation	Continued
	Chem i	Med j	Effect l				$S_{iml}, B_{iml}, b_{iml}$													
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-5

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS
V. Emission/Effluent Rates

Case Code
73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units									Uncertainty Codes		Documentation	Continued
Q	Chem i	Loc j	Med m				Q_{ijm}									+ or -		b or %		
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-6

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS
VI. Air Pollutant Model – Concentration Multipliers

Case Code
73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units								Uncertainty			Documentation	Continued
SMC	Chem i	Loc j	Pop Type n	Pop Index k			c_{ijnk}									+ or -	Codes	b or %		
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-7

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS

VII-A Water Pollutant Model – Flow Rates and Transit Times

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units												
SMF SMT	Loc j	Pop Type n	Pop Index k				f_{jnk}, t_{jnk}									+ or −	Uncertainty Codes	b or %	Documentation	Continued
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-8

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS
VII-B Water Pollutant Model – Transformation-Transfer Rates

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units									Uncertainty Codes		Documentation	Continued
LMD	Chem i	Med m H20					λ_{im}									+ or •		b or %		
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-9

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS

VII–C Water Pollutant Model – Purification Factors

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units								Uncertainty Codes			Documentation	Continued
R	Chem i	Pop Type n					R_{in}									+ or -		b or %		
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-10

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS

VIII-A Ground Water Pollutant Model – Diffusion Constants and Flow Rates

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units								+ or −	Uncertainty Codes	b or %	Documentation	Continued
D SMV	Chem i	Loc j					D_{ij}, v_{ij}													
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-11

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS

VIII-B Ground Water Pollutant Model – Locations of Wells and Ground Water Outfalls

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value		Units									Uncertainty Codes		Documentation	Continued
ZX	Chem i	Loc j	Pop* Type n	Pop Index k			Z_{ijnk}	X_{ijnk}									+ or −		b or %		
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27	28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27	28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

*For ground water outfall, code GWO.

FIGURE A.C-12

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS

VIII-C Ground Water Pollutant Model – Transmissivity, Gradient, and Length of Ground Water Outfalls

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units												
TR SMG L	Loc j	Outfall Index k					TR_{jk}, g_{jk}, L_{jk}									+ or -	Uncertainty Codes	b or %	Documentation	Continued
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-13

AMRDC POLLUTANT HAZARD MODEL DATA SHEETS

IX Concentrations

Case Code

73 74 75 76 77 78 79 80

Variable	Subscripts						Value	Units												
C	Chem i	Loc j	Med m	Pop Type n	Pop Index k		C_{ijmnk}									+ or -	Uncertainty Codes	b or %	Documentation	Continued
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24 25 26 27 28 29 30 31 32	33	34 35 36	37	38 39 40	41	42 43 44	45	46 47 48	49	50 51 52 53 54	55	56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

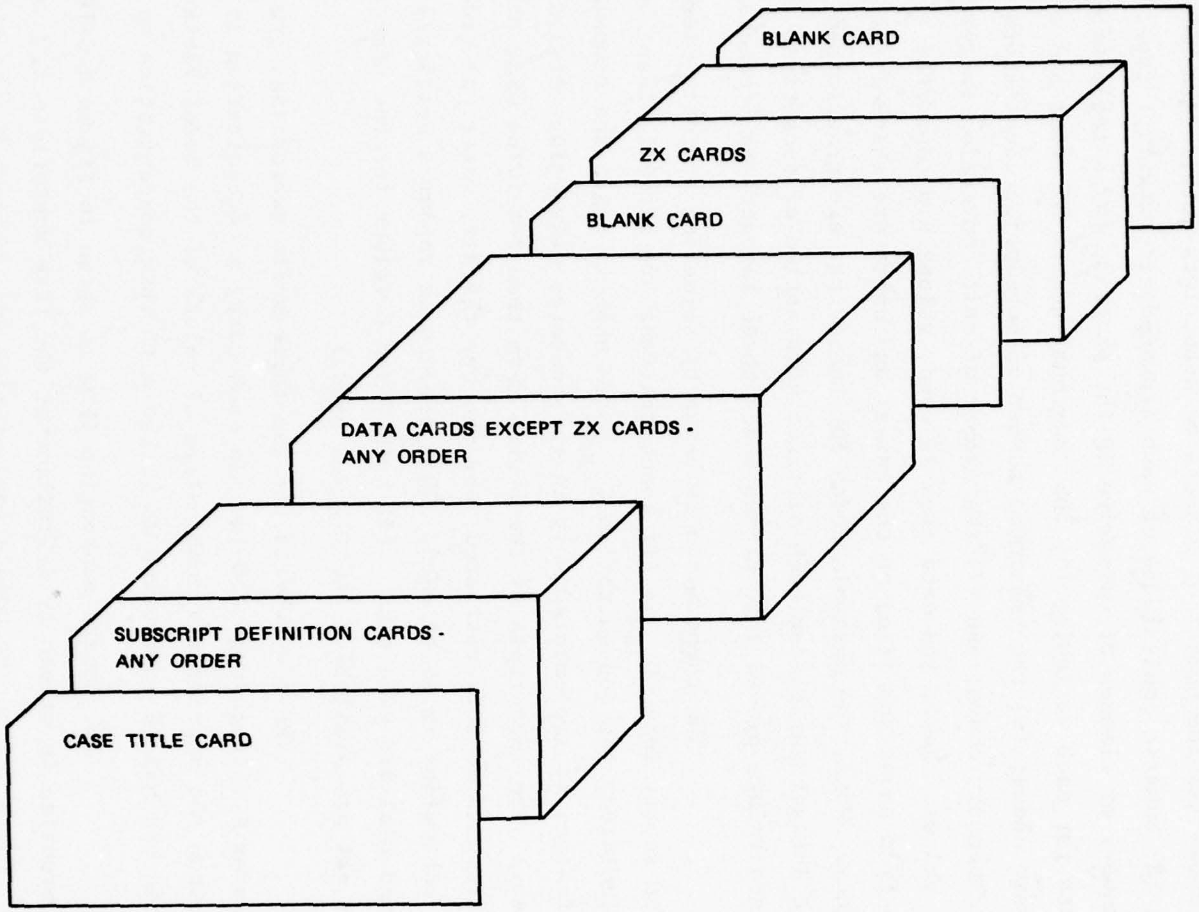

FIGURE A.C-14 BATCH INPUT DATA DECK

A.C.1.3 Program Flow

The overall flow of the hazard estimating program is shown in Figure A.C-15. The first operation is to read in a table of values that shows (1) the number of classes of subscripts (other than MED and PID); (2) numeric equivalents of each alphanumeric subscript type; (3) the number of classes of variables in the program; (4) a table of subscripts for each variable; (5) the (maximum) number of media and their mnemonic codes; (6) the (maximum) number of population identifiers and their mnemonic codes; and (7) the number of unit conversion factors and their values. Next, the data deck is read, values are converted to CGS units from those specified on the cards, and units are checked for consistency. Next, the mnemonic codes for subscripts are transformed into unique integer values for each distinct combination of subscripts and the data values placed into tables using these integers as locators.

The computation is begun by selecting any data element for the source term, Q_{ijm}. (If concentrations are directly input instead of calculated, the concentration C_{ijmnk} is used to begin the computation. This feature is implemented only in the resource allocation version of the program.) The subscripts of the source term then determine what other data elements must be retrieved, and whether the air, water, or groundwater subroutine is to be used. This process is repeated until all the Q's (and C's) are exhausted. (If both Q and C values for the same subscript set are available, the C's are used.)

The flow charts for the three media subroutines are shown in Figures A.C-16 through A.C-18. In each case, a concentration is calculated from the appropriate combination of values of the model variables and then the hazard subroutine is called with this concentration as input.

The hazard subroutine flow is shown in Figure A.C-19. The subroutine is driven by definition of the five subscripts i, j, m, n, and k. These define the populations-at-risk and, through V, the effects under consideration. The principal computation of HAZARD is a six-subscript hazard value, in \$/yr; these are then combined into aggregated hazards by chemical and location for printing in a summary table.

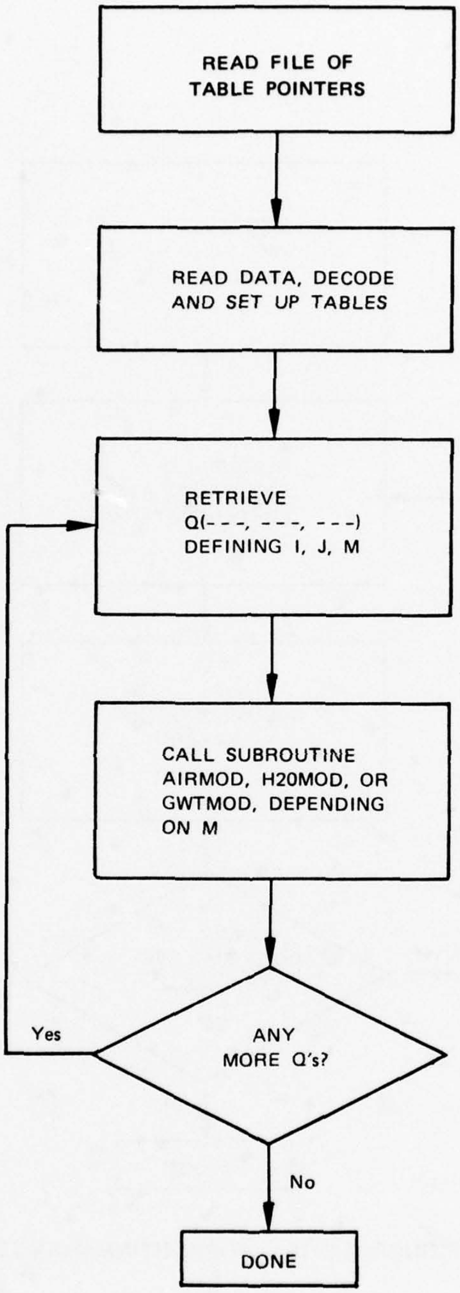

FIGURE A.C-15 PROGRAM FLOW FOR HERS

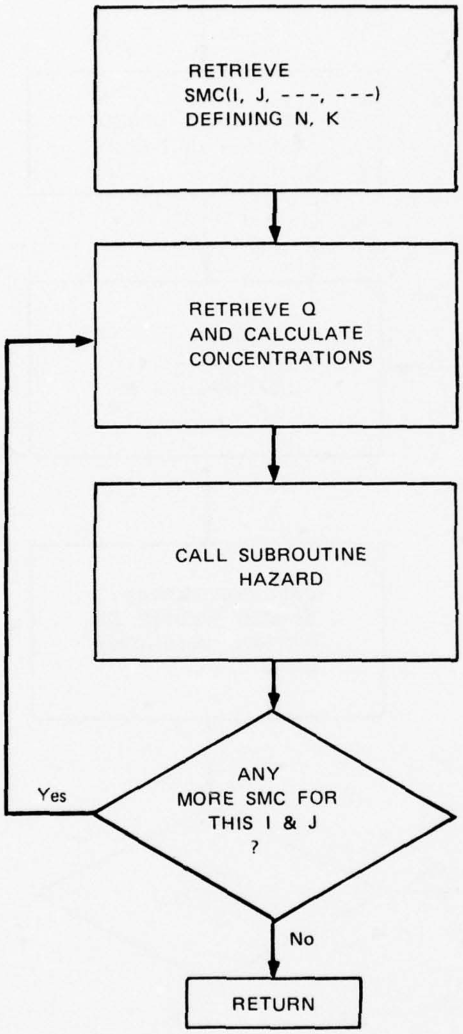

FIGURE A.C-16 SUBROUTINE AIRMOD

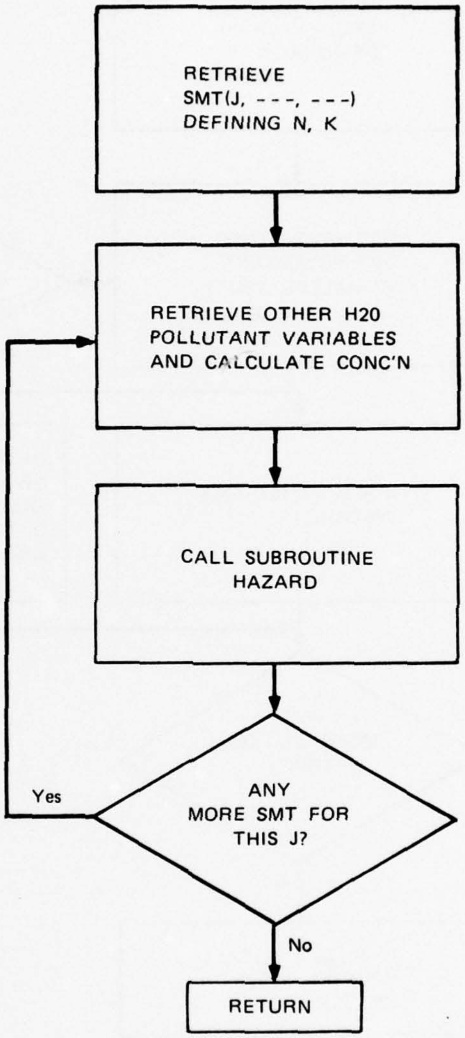

FIGURE A.C-17 SUBROUTINE H20MOD

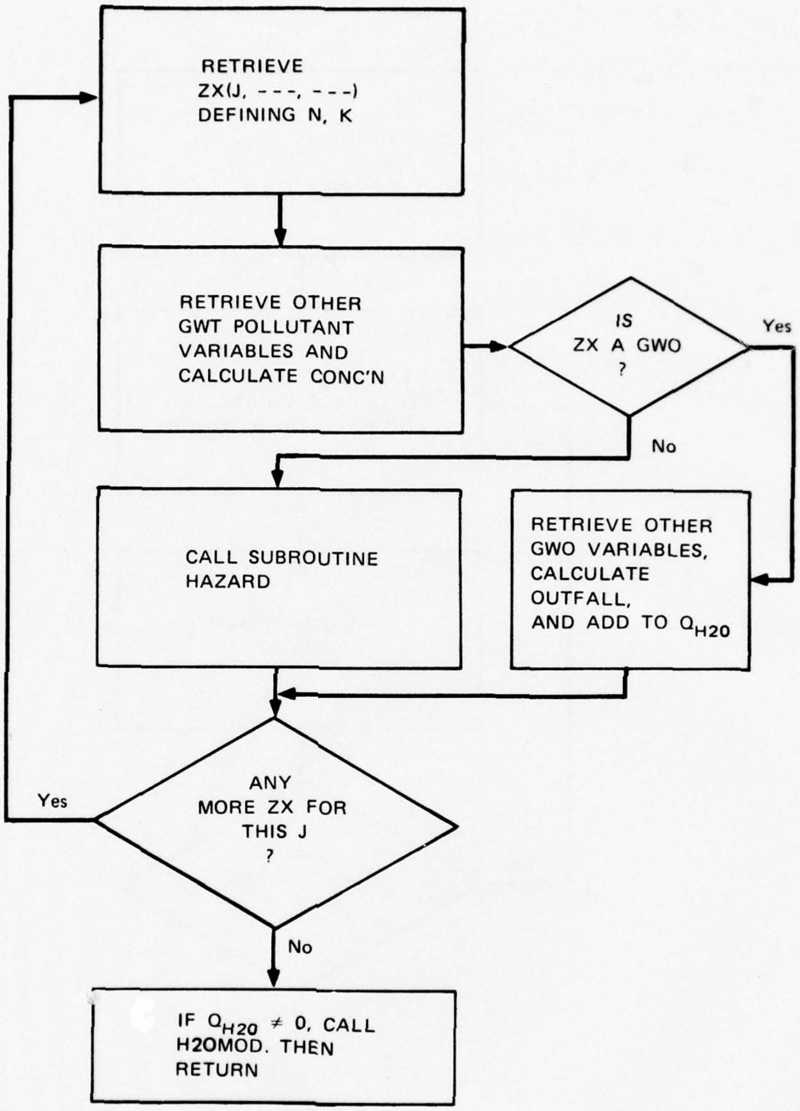

FIGURE A.C-18 SUBROUTINE GWTMOD

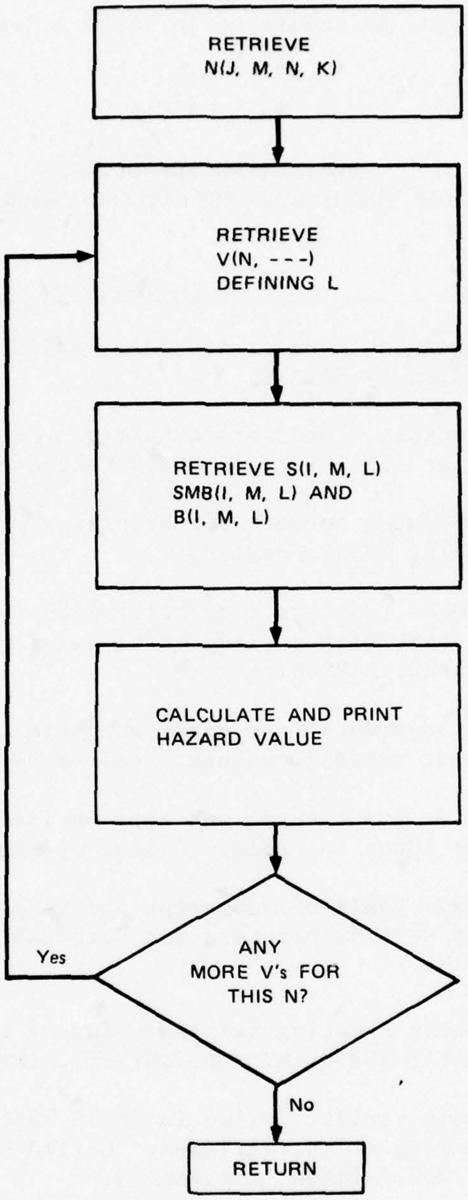

FIGURE A.C-19 SUBROUTINE HAZARD

Besides the main program and the AIRMOD, H2OMOD, GWTMOD, and HAZARD subroutines, there are a number of specialized subroutines that perform functions as tabulated in Table A.C-6.

Table A.C-6

SPECIALIZED SUBROUTINES
OF THE HAZARD ESTIMATING PROGRAM

Name	Function
ADDUN	Checks that units of added variables are the same. Called by HAZARD.
MODEL	Acquires Q and sets subscripts used. Chooses between AIR, H2O, and GWT. Called by MAIN.
MOVE	Generates formats for printing. Called by WRPRTS, RDATA, MODEL, HAZARD.
MULTUN	Checks that units of multiplied variables are consistent with desired results. Called by MAIN, HAZARD, AIRMOD.
RDATA	Decodes data from cards and sets up table of all input variable values. Called by MAIN.
RDCARD	Reads input cards and sets up intermediate arrays for input to table. Called by RDATA.
RDTBLS	Reads table of subscript and variable definitions and sets up pointers for data table. Called by MAIN.
SEARCH	Speeds creating and searching of table. Called by RDATA, MODEL, H2OMOD, GWTMOD, AIRMOD, HAZARD.
SEEK	Finds variable value in table based on subscripts needing to be retrieved. Called by MODEL, H2OMOD, GWTMOD, AIRMOD, and HAZARD.
SORTAG	Sorts a group of values into descending order. Used to create tables. Called by RDATA.
WRPRTS	Generates report on aggregate hazards by chemical and location. Called by MAIN.

A.C.2 The Resource Allocation Program

The resource allocation program (AMRDCP) implements the uncertainty propagation and reduction models discussed in Section A.7, using the equation shown in Section A.7.3.

A.C.2.1 Program Specifications

The complete hazard estimating program* is incorporated in the resource allocation program, so that the six subscript hazards may be calculated. Additionally, the uncertainty in each input variable value is read and kept with the value itself at every step of the process.

An overview of the computer program is given in Section A.7.4.1. The basic inputs, in addition to the hazard data described earlier, are the number of Monte Carlo simulations to be done (up to 100 for an overnight run), which is currently a programmed input, and the research study data, which specify the aggregate hazard to be evaluated and the uncertainties and cost associated with each study.

The choice of the exact number, NRSAMP, of simulations to perform depends on the tradeoff between computer costs and acceptable accuracy. If NRSAMP is too low, then a number of candidate studies will show too high or too low a difference in standard deviation, even to the point of showing a spurious negative difference. (In the printout, negative differences are shown as 0.*. These should be checked to see if the input data show an absolute increase in uncertainty, in which case the data should be revised or the study dropped from consideration.) The spurious negatives should be removed by going to more iterations; however, a spurious negative is more likely to occur when the difference in standard deviation is small relative to the two standard deviations. Studies with little change in uncertainty are often not very attractive for selection in any case.

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*Including direct concentration input.

The only totally new input variable for the resource allocation program is the cost of a project in a study, C_p. The other input is simply the uncertainty in a specified variable expected after a project is complete.

The program makes two passes through the hazard program for each Monte Carlo step. On the first pass, the best estimate of an input variable and its uncertainty estimate are combined with a random number to produce a sample value for the variable. All such sample values are combined into the six subscript hazards, and aggregated according to the rules discussed in Section A.7.3.2. In the second pass, the variable whose uncertainty is affected is singled out, and a new sample value is generated from the new uncertainty, leaving the best estimate and random number alone. The hazards are again calculated and aggregated. This subsequent hazard pass is repeated for each candidate study. A previously-altered sample value is returned to its prior case value after each study is evaluated.

Registers are set up for H and H^2 for each prior and each subsequent aggregate hazard as defined by each project. These registers sum H and H^2 for statistical analysis.

A.C.2.2 Data Inputs

The data input coding sheet for the resource allocation program is presented as Figure A.C-20. Only the subscripts that apply to the variable(s) affected by a project are entered. If the variable does not contain a given subscript, the code is left blank. If all variables of the same type are to be determined, the code is set to XXX.* Project costs in whole dollars are entered "right-justified" in columns 28-34. No unit input is required. Uncertainty codes are as described earlier. Program codes are shown in Table A.7-2. Program Title is shown as one

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*At the time of writing, the XXX code is recognized as equivalent to a blank code.

AMRDC RESEARCH PROGRAM PRIORITIES DATA SHEET
(Programs, *Variables Affected, Costs, and Effectiveness*)

Vari-able PRØ	Sub-script Prog P	Vari-able Afft'd	Subscripts Affected						Program Cost (dollars)	+ or •	Uncertainty Code After Program	b or %	Program Title	Documentation	
			Chem i	Loc j	Med m	Pop Type n	Pop Index k	Effect l							
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24	25 26 27	28 29 30 31 32 33 34	35	36 37 38 39 40	41	42 43 44 45 46 47 48 49 50 51	52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72
1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24	25 26 27	28 29 30 31 32 33 34	35	36 37 38 39 40	41	42 43 44 45 46 47 48 49 50 51	52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71	72

FIGURE A.C-20 AMRDC RESEARCH PROGRAM PRIORITIES DATA SHEET (PROGRAMS, VARIABLES AFFECTED, COSTS, AND EFFECTIVENESS)

10-character word for 60-bit machines; this could be changed to three 4-character words for a 24-bit machine if desired. The documentation field is used as for the hazard estimating program, and can be continued if desired.

After the input cards are punched, the deck is inserted between the table deck and the data deck. Order within this deck is also unimportant for these cards.

A.C.2.3 Program Flow

The general features of the resource allocation program flow are shown in Figures A.7-6 through A.7-8. Figure A.C-21 shows these flows somewhat more accurately from the program operator's point of view. The blocks containing the phrase "(re)compute aggregate hazard" incorporate virtually all of the operations of the HERS program.

The number of studies read into the files determine how many registers need to be set up to keep track of the Monte Carlo results. The total number of data elements (variable values) read in determines how many random numbers need to be generated. The sample value, X_s, of a variable X is computed as

$$X_s = \hat{X} e^{r_s \sigma_X}$$

where $\hat{X}$ is the best estimate of X, σ_X is the standard deviation of X, and r_s is the randomly-selected value from the (0,1) normal distribution. (See Figures A.7-4 and A.7-7.)

The determination of the six subscript hazards to constitute the aggregate hazard is done in the modified subroutine MODEL by testing the subscripts in the study cards against those in the data base. Computation of sample hazards is then done essentially as in the hazard estimating system.

Changing the sample variable value to the subsequent case and then resetting it is done in the main program.

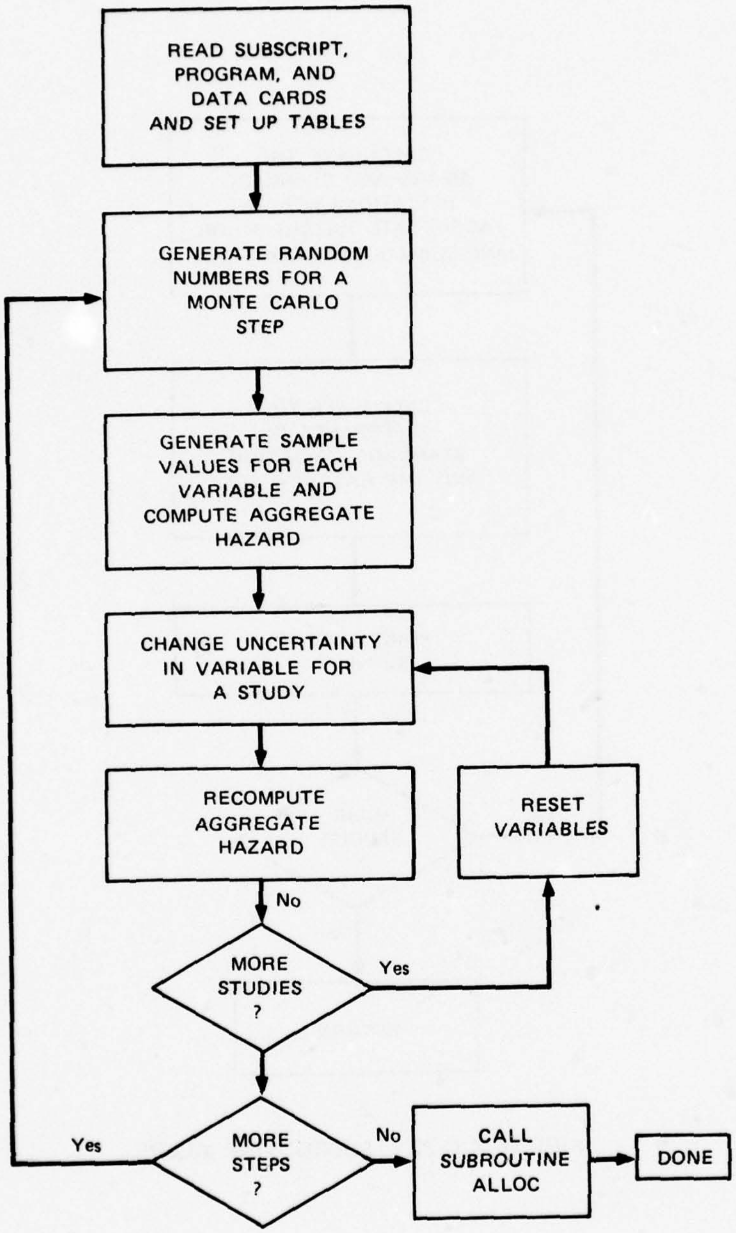

FIGURE A.C-21 ALLOCATION PROGRAM FLOW

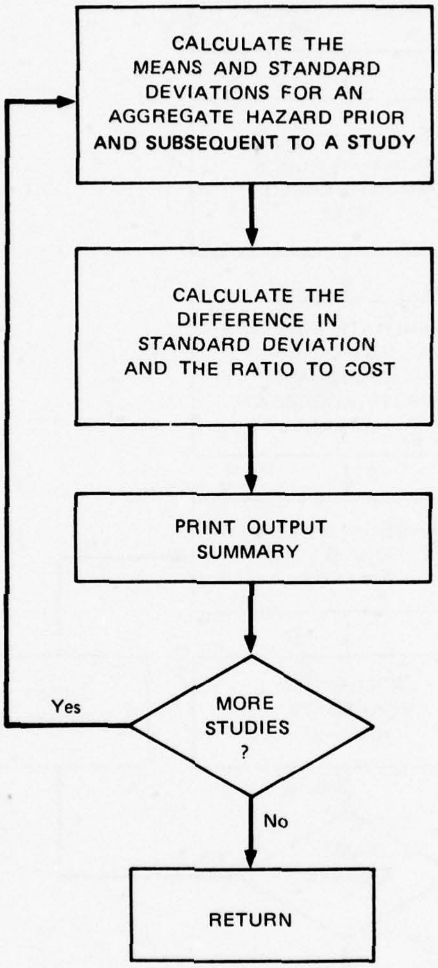

FIGURE A.C-22 SUBROUTINE ALLOC

The principal new subroutine of AMRDCP in comparison with HERS is ALLOC. The ALLOC subroutine flow is shown in Figure A.C-22. Besides doing the calculations shown, the subroutine checks for negative $\Delta\sigma$'s and replaces them with 0, showing an asterisk as a marker.

The other specialized subroutines added to those of the hazard estimating program are tabulated in Table A.C-7.

Table A.C-7

SPECIALIZED SUBROUTINES
OF THE RESOURCE ALLOCATION PROGRAM

Name	Function
GGNOF (Function)	Generates normal (0,1) pseudo-random number. Called by MAIN
MERFI, UERTST	Associated with GGNOF.
RPROGS	Reads program (study) cards, processes uncertainty, and checks for XXX. Called by MAIN.

A.C.3 Auxiliary Programs

The only auxiliary program in use at the time of writing was CDM.

A.C.3.1 The Climatological Dispersion Model

This program is documented both by EPA (1973) and by Whitby and Bun (Bun 1976a). The general features of the model are described in Section A.B.2.2. CDM requires considerable quantities of carefully prepared input data. The input formats are described in Table A.C-8.

Table A.C-8

INPUT FORMATS FOR SRI VERSION OF CDM PROGRAM

Card	Column	Format	Contents
1	1 to 8	2A4	AROS(1)-AROS(2) (Identification for punched output of the computed area source concentrations of the two pollutants. See sample punched output.)
	9 to 16	2A4	PROS(1)-PROS(2) (Identification for punched output of the computed point source concentrations of the two pollutants.)
	17 to 21	I5	IRUN (Computer run identification number.)
	22 to 26	I5	NLIST (Index which indicates whether input data should be listed. If NLIST ≤ 0, input data is printed.)
	27 to 31	I5	IRD (card input file number)
	32 to 36	I5	IWR (Output print file number)
	37 to 41	I5	IPU (Output punch file number)
	42 to 59	2F9.0	CA(1)-CA(2) (Constants of the linear equation Y = CA + CB x X, used to calibrate the calculated concentrations of the two pollutants considered in the model)
	60 to 77	2F9.0	CB(1)-CB(2) (Slope of the linear equation, Y = CA + CB x X, used to calibrate the calculated concentrations of the two pollutants considered in the model)
2-1	1 to 6	F6.0	DELR (Initial integration increment of radial distance from receptor, meters)
	7 to 12	F6.0	RAT (Ratio of length of a basic emission grid square and the length of a map grid square)
	13 to 18	F6.0	CV (Conversion factor which upon multiplication by RAT expresses the distance of the side of an emission grid square in meters. For example, if the map units are in kilometers, CV = 1000.)

Table A.C-8 (Continued)

Card	Column	Format	Contents	
2-1 (Cont.)	19 to 24	F6.0	HT(1) (Average afternoon mixing height in meters, season 1)	
	25 to 30	F6.0	HMIN(1) (Average nocturnal mixing height in meters, season 1)	
	31 to 36	F6.0	XG (X map coordinate of the southwest corner of the emission grid array)	
	37 to 42	F6.0	YG (Y map coordinate of the southwest corner of the emission grid array)	
	43 to 48	F6.0	XGG (X map coordinate of the southwest corner of the plotting grid)	
	49 to 54	F6.0	YGG (Y map coordinate of the southwest corner of the plotting grid)	
	55 to 60	F6.0	RATG (Ratio of the length of the grid square used for plotting and the length of a map grid square)	
	61 to 66	F6.0	TØA(1) (Mean atmospheric temperature in degrees centigrade, season 1)	
	67 to 72	F6.0	TXX (Width of basic emission square in meters)	
Three 2-2 cards	1 to 6	F6.0	HT(i) (Average afternoon mixing height in meters)	For seasons i=2 through 4
	7 to 12	F6.0	HMIN(i) (Average nocturnal mixing height in meters)	
	13 to 18	F6.0	TØA(i) (Mean atmospheric temperature in degrees centigrade)	
3	1 to 6	F6.0	DINT (Number of intervals used to integrate over a 22.5° sector. Maximum value is 20, typical value is 4.)	
	7 to 12	F6.0	YD (Ratio of average daytime emission rate to the 24-hour emission rate average)	

Table A.C-8 (Continued)

Card	Column	Format	Contents
3 (Cont.)	13 to 18	F6.0	YN (Ratio of the average nighttime emission rate to the 24-hour emission rate average)
	19 to 54	6F6.0	SZA(1)-SZA(6) (Initial σ_z in meters for each stability class. Six different values can be used, bur normally only one value is used.)
	55 to 66	2F6.0	GB(1)-GB(2) (Decay half-life in hours for the two pollutants)
Four blocks of 96 cards each	1 to 63	[9X,6(1X, F8.6)]	F(i,j,k) (Joint frequency function, identical to $\phi(k,\ell,m)$; i = index for stability class, j = index for wind speed, k = index for wind direction. See input data of sample problem for proper ordering of this parameter by stability class, wind direction, and wind speed. One block of 96 cards for each seasons.
(Source cards follow)	1 to 6	F6.0	X (X map coordinate of the southwest corner of the area emission grid, or if appropriate, the X map coordinate of a point source)
	7 to 13	F7.0	Y (Y map coordinate of the southwest corner of the area emission grid, or if appropriate, the Y map coordinate of a point source)
	14 to 20	F7.0	TX (Width of an area grid square in meters. It is important that no entry be made in the case of a point source.)
	21 to 36	2F8.0	S1-S2 (Source emission rate in grams per second for the two pollutants)
	37 to 43	F7.0	SH (Stack height in meters)
	44 to 48	F5.0	D (Diameter of stack in meters)
	49 to 55	F7.0	VS (Exit speed of pollutants from stack in meters per second)

Table A.C-8 (Concluded)

Card	Column	Format	Contents
(Source) (Cont.)	56 to 62	F7.0	T (Gas temperature of stack gases in degrees centigrade)
	63 to 67	F5.0	SA (If this field is blank, Briggs' formula is used to compute stack height. Otherwise, the product of plume rise and wind speed is entered in square meters per second.)
	--	--	This is a blank card which follows information on the emission sources. It is used to test the end of sources and must not be left out.
(Receptor cards follow)			
	1 to 8	F8.2	RX (X map coordinate of the receptor)
	9 to 16	F8.2	RY (Y map coordinate of the receptor
	31 to 34	I4	KPX(9) (Observed concentration at the receptor of the first pollutant)
	38 to 41	I4	KPX(10) (Observed concentration at the receptor of the second pollutant)
	42 to 46	I5	NROSE (A control that, if greater than zero, will print out histogram concentration data. If left blank, no histogram data will be printed.)
	47 to 58	3A4	REC (Name of receptor location)
	59 to 63	I4	IPØP (Population affected at receptor location)

A.D. CIVILIAN CHEMICALS

Comparison of the hazards of Army chemicals with the hazards of civilian chemicals is desirable from the point of view of placing the Army's problems in perspective with the nation's problems. However, the widespread nature of civilian production and use makes this difficult in practice. A compromise approach was taken in which five sample civilian chemicals were selected from a list previously generated by SRI for the National Science Foundation (SRI 1975). These five are benzene, nitrobenzene, polyvinyl chloride (PVC manufacturing as a source of vinyl chloride monomer), carbon tetrachloride, and dichlorodifluoromethane (one of the aerosol propellants and refrigerants).

As these chemicals are produced at multiple locations, two large representative plants were selected for processing through the ranking system. The plants were presumed to be operating at a production level proportionate to their share of the total reported capacity. Hazards were calcualted at these levels, and then scaled up to total reported production. Most data came from the NSF study of manufactured organic chemicals (SRI 1975). However, data on populations-at-risk and transport media were developed. One difficulty with civilian chemicals is that many of the production sites are coastal, and no methodology for such sites has been developed.

Civilian production levels for a wide variety of chemicals also produced or used by the Army were determined to the extent such levels were available. A summary of the findings is presented in Tables A.D-1 and A.D-2, followed by references.

Table A.D-1

CIVILIAN PRODUCTION AND USE OF THE EPRD CHEMICALS OF CONCERN

	Chemical	Estimated 1973 Production (millions of pounds)	Uses
1.	Nitroglycerine	at least 58 (1)	Ingredient in explosives and some propellant compositions (2), (3)
2.	2,4- and 2,6- Dinitrotoluene	471 (4)	Gelatinizing and waterproofing agent in explosive compositions; used to produce toluene diamine, an intermediate in the manufacture of toluene diisocyanate (2)
3.	Trinitrotoluene	N.P.	Non-initiating high explosive; used in bombs and grenades (2)
4.	Nitroguanidine	N.P.	Found to have value as propellant for anti-aircraft guns (5)
5.	Trinitroresorcinol	N.A. (6)	Intermediate in the manufacture of lead styphnate (6)
6.	Tetracene	N.P.	Ingredient for priming compositions (7)
7.	Lead styphnate	N.A. (8)	Ingredient in priming mixture for civilian production of ammunition (8)
8.	Tetryl	N.P. (9)	Has been used as a booster explosive and as an ingredient of formulated binary explosives (10)
9.	PETN (Pentaerythritol tetranitrate)	5 (11)	An explosive used as a filling in detonating cord and detonators (2), (12)
10.	Phosphorus (white)	1,052 (2)	Used to manufacture phosphoric acid and other phosphorus compounds (2)

N.P. = Not produced for civilian purposes

N.A. = Information is not available

Table A.D-1 (Continued)

	Chemical	Estimated 1973 Production (millions of pounds)	Uses
11.	RDX (Cyclonite)	N.P. (6), (13)	High explosive; has been used as an ingredient of bursting charge and plastic explosives (14),(15)
12.	HMX (Cyclotetramethylenetetranitramine)	N.P.	Is formed in the course of cyclonite production (16)
13.	Methyl nitrate	N.P.	Has been investigated as an ingredient in a monopropellant mixture (17)
14.	Tetranitromethane	very small, custom manufacture (9)	For research purposes; has been used as an oxidizer in rocket propellants (9), (15)
15.	Nitromethane	1 (13)	Auto racing fuel additive; some usage as an intermediate (13)
16.	Nitrotoluenes (o, m, p-)	o- 20 m- 13.5 (18) p- 1.3	Are used to produce dye intermediates (e.g. toluidines) and as ingredients in production of explosive compostitions (2)
17.	Mustard gas	very small, laboratory quantities (19)	Has been tested as an anti-neoplastic agent; Is used as a model compound in biological studies on alkylating agents; Was used as a vesicant in World War I (19)
18.	Thiodiglycol (2,2'-Thiodiethanol)	3 (20)	Used for the treatment of synthetic fabrics prior to printing or dyeing (20)
19.	Lewisite (Arsine, Dichloro(2-Chlorovinyl)-)	N.P.	Poison gas and blistering agent (15)
20.	Lewisite oxide	N.P.	Degradation product of lewisite
21.	Methyl phosphonic acid	very small, research purposes only (21)	Organic synthesis research (21), (22)
22.	Isopropylmethylphosphonate	N.P.	Degradation product of GB (isopropyl methylphosphonofluoridate) a nerve gas

N.P. = Not produced for civilian purposes

N.A. = Information is not available

Table A.D-1 (Continued)

	Chemical	Estimated 1973 Production (millions of pounds)	Uses
23.	Diisopropylmethylphosphonate	N.P.	Degradation product of GB
24.	Mercury	0.94 (23) (3.50 - imports)	Electrical apparatus; Electrolytic preparation of chlorine and caustic soda; Paint; Industrial and control instruments; Dental preparations; pesticides (23)
25.	Dicyclopentadiene	96 (24) (includes cyclopentadiene)	Intermediate for pesticides, fire retardant resins, and EPDM elastomers (25)
26.	Aldrin	13 (26)	Insecticide used on corn crops and for termite control, (27). Suspended Aug. 1974. Shell discontinued production and sales in the U.S.
27.	Chlordane	20 (26)	Insecticide for ants, roaches, and termites and on lawn and corn soil insects (28) Suspended as of Dec. 1975 for most agricultural and home usage. Termite use is still allowed.
28.	Dieldrin	2^* (29) (1974)	Insecticide for corn crops and termite control. Suspended Aug. 1974. Shell discontinued production and sales in the U.S. (30)
29.	Endrin	6 (29) (1974)	Insecticide approved for use on seven agricultural crops; rodenticide; avicide (31)
30.	Glycerol-1,3-dinitrate	N.P.	N.A.
31.	Glycerol-1-nitrate	N.P.	N.A.
32.	Glycerol-2-nitrate	N.P.	N.A.
33.	Chromium (as chromic acid)	60 (2)	Used in metal treatment for chrome plating, copper stripping and aluminum anodizing. Also used for catalysts, refractories and as an oxidizing agent in the production of dyes and organic chemicals (2)

N.P. = Not produced for civilian purposes N.A. = Information is not available
* = 1974 production figure is much lower than 1973 since it was suspended during 1974.

Table A.D-1 (Continued)

	Chemical	Estimated 1973 Production (millions of pounds)	Uses
34.	2-Chlorovinylarsonic acid	N.P.	Degradation product of lewisite
35.	Diisopropyldimethyldiphosphonate	N.P.	Degradation product of GB
36.	Cadmium	7.428 (23)	Used for electroplating, in cadmium compounds, in nickel-cadmium and silver-cadmium batteries, alloys, and cadmium phosphors (23)
37.	Chlordene	N.P.	Intermediate in the production of chlordane but is not isolated and sold as such (25)
38.	Heptachlor	6 (29)	Insecticide for termite control and on corn and other vegetables. Suspended as of Dec. 1975 for most agricultural and home usage. Termite use is still allowed (32)
39.	Heptachlor epoxide	N.P.	Degradation product of heptachlor
40.	Nudrin	over 5 million (29) (1974)	Insecticide registered for use on 25 agricultural crops (32)
41.	Azodrin	5.3 (29) (1974)	Insecticide for cotton plants (33), (22)
42.	Bidrin	1.0 (29) (1974)	Insecticide and acaricide registered for use on cotton, soybeans (raised for seed), several ornamental plants and shrubs, trees, and vines (33)
43.	Ciodrin	1.25 (29) (1974)	Insecticide for livestock to control flies, lice, and ticks (33)
44.	Phosdrin	0.85 (29)	Systemic insecticide and acaricide used on the foliage of various agricultural crops (33)

N.P. = Not produced for civilian purposes

N.A. = Information is not available

Table A.D-1 (Continued)

	Chemical	Estimated 1973 Production (millions of pounds)	Uses
45.	Dimethyl phosphate	N.P.	Hydrolysis product of phosdrin
46.	Nemagon	10 (34) (1971)	Soil fumigant used on a variety of crops for nematode control (33)
47.	Hexachlorocyclopentadiene	N.A.	Intermediate for pesticides (cyclodiene insecticides), fungicides, resins, dyes, and pharmaceuticals (35), (22)
48.	Methyl acetoacetate	N.A. (36) (proprietary)	Solvent for cellulose ethers; ingredient of solvent mixtures for cellulose esters; organic intermediate (22)
49.	Trimethyl phosphite	1 (25) (1972)	Chemical intermediate, especially for insecticides (22)
50.	Trimethyl phosphate	N.P.	Was used as a gasoline additive for controlling spark plug fouling, surface ignition, and rumble (22)
51.	Methyl 2-chloroacetoacetate	N.A.	N.A.
52.	Allyl chloride	334 (29)	Chemical intermediate in the synthesis of glycerin and epichlorohydrin (25)
53.	Allyl alcohol	N.A. (37) (proprietary)	Primary use as an intermediate in the manufacture of flame retardant chemicals and as a cross-linker in polymerization (37)
54.	Heptachlorobicycloheptane	N.P.	N.A.
55.	Hexachlorobicycloheptadiene	N.P.	Was used to make isodrin (38)
56.	Isodrin	N.P.	Isomer of aldrin which was never commercially produced in the U.S. (33)

N.P. = Not produced for civilian purposes

N.A. = Information is not available

Table A.D-1 (Continued)

	Chemical	Estimated 1973 Production (millions of pounds)	Uses
57.	Bicycloheptadiene	N.P.	N.A.
58.	Sodium chlorate	347 (2)	An ingredient used to make chlorine dioxide for bleaching kraft pulp and paper; to manufacture chlorates and perchlorates; used as a herbicide for weed control (2)
59.	Calcium chlorate	Very small (39) (research purposes only)	Has been used in photography; pyrotechnics; and as a dusting powder to kill poison ivy (22)
60.	Potassium chlorate	7 (40)	Primarily used in the manufacture of match tips (40)
61.	Arsenic trioxide	23 - Imports *U.S.* production *is* not disclosed (2)	Used in the manufacture of pesticides; glass; *industrial inorganic* chemicals; non-ferrous alloys; pharmaceuticals (2)
62.	Arsenic trichloride	N.A.	Intermediate for organic arsenicals (pharmaceuticals, insecticies); ceramics (22)
63.	Trimethyl arsine	N.P.	Is produced when certain molds are allowed to grow on a suitable substrate containing arsenic (III) oxide (41)
64.	Mercuric oxide	N.A.	A starting material for the preparation of various mercury compounds; Has been used in medicines, antiseptics, fungicides, germicides and as an ingredient of anti-fouling paints. Is also used as a depolarizer in mercury batteries (44)
65.	Mercuric chloride	N.A.	Has been used as a fungicide, disinfectant, and sterilizing agent, to preserve wood, and as a catalyst in many organic chemical processes. Has also been used in the treatment of underexposed photographic negatives (44)

N.P. = *Not produced for civilian purposes*

N.A. = *Information is not available*

Table A.D-1 (Concluded)

	Chemical	Estimated 1973 Production (millions of pounds)	Uses
66.	Cuprous chloride	1.5 (42)	Primarily used in the production of inks and organic colors (42)
67.	4-Amino-2,6-dinitrotoluene	N.P.	N.A.
68.	2-Amino-4,6-dinitrotoluene	N.P.	N.A.
69.	Nitrodiphenylamine	N.A.	Has been used as an intermediate. Has also been used as a stabilizer in certain propellant compositions (22), (45)
70.	Glycerol-1,2-dinitrate	N.P.	N.A.
71.	Cyclohexone	N.P.	N.A.
72.	Hexamine (Hexamethylenetetramine)	100 (43)	Main use is in the production of trimethylene trinitramine which is used to make cyclonite explosive. Second largest use is in phenolic thermosetting-resin cure agents (2)
73.	SEX	N.P.	N.A.

N.P. = Not produced for civilian purposes

N.A. = Information is not available

Table A.D-2

1973 CIVILIAN MANUFACTURERS AND PLANT LOCATIONS OF ARMY CHEMICALS OF CONCERN

Chemical	Company	Plant Location
1. Nitroglycerine	E.I. du Pont de Nemours and Co., Inc. Polymer Intermediates Dept.	Du Pont, WA Martinsburg, WV
	Hercules Inc. Indust. Systems Dept.	Bessemer, AL Carthage, MO* Kenvil, NJ*
2. 2,4-Dinitrotoluene	Air Products and Chems. Inc.	Pensacola, FL
	E.I. du Pont de Nemours and Co., Inc. Organic Chems. Dept.-Dyes and Chems. Div.	Deepwater, NJ
	Rubicon Chems. Inc.	Geismar, LA
2,4- and 2,6-	Mobay Chem. Corp. Indust. Chems. Div.	Cedar Bayou, TX New Martinsville, WV
3. 2,4,6-Trinitroresorcinol	Northrop Corp. Northrop Carolina, subsid.	Asheville, NC
	Olin Corp. Winchester-Western Div. Energy Systems Operations	East Alton, IL
4. Lead styphnate (Styphnic acid, lead salt)	Remington Arms Co., Inc.	Bridgeport, CT
5. PETN (Pentaerythritol tetranitrate)	Commercial Solvents Corp. Trojan-U.S. Powder Div.	Seiple, PA
	E.I. du Pont De Nemours and Co., Inc. Polymer Intermediates Dept.	Louviers, CO
	Hercules Inc. Indust. Systems Dept.	Kenvil, NJ*

Table A.D-2 (Continued)

	Chemical	Company	Plant Location
6.	Phosphorus	FMC Corp. Inorganic Chems. Div.	Pocatello, ID
		Holmes Co., Inc.	Pierce, FL
		Mobil Oil Corp. Mobil Chem. Co., Div. Indust. Chems. Div.	Nichols, FL
		Monsanto Co. Monsanto Indust. Chems. Co.	Columbia, TN Soda Springs, ID
		Occidental Petroleum Corp. Hooker Chem. Corp., subsid. Electrochemical and Specialties Divisions	Columbia, TN
		Stauffer Chem. Co. Indust. Chem. Div.	Mt. Pleasant, TN Silver Bow, MT Tarpon Springs, FL
		Tennessee Valley Authority	Muscle Shoals, AL
7.	RDX (Cyclonite)	Olin Corp. Winchester Western Div. Energy Systems Operations	East Alton, IL*
8.	Tetranitromethane	Hummel Chem. Co., Inc.	South Plainfield, NJ
9.	Nitromethane	Commercial Solvents Corp.	Sterlington, LA
10.	Nitrotoluenes o-, m-, and p-	E.I. du Pont de Nemours and Co., Inc. Organic Chems. Dept. Dyes and Chems. Div.	Deepwater, NJ
		First Mississippi Corp. First Chem. Corp., subsid.	Pascagoula, MS

Table A.D-2 (Continued)

	Chemical	Company	Plant Location
11.	Thiodiglycol (2,2'-Thiodiethanol)	Union Carbide Corp. Chems. and Plastics Div.	Institute and South Charleston, WV
		Witco Chem. Corp. Argus Chem. Corp., subsid. Halby Div.	Le Moyne, AL
		Pierce Chem. Co.	Rockford, IL*
12.	Methyl phosphonic acid	Frank Enterprises	Columbus, OH
13.	Mercury	The reader should refer to the <u>1973 Minerals Yearbook</u> to obtain his own interpretation of this metal's mining status.	
14.	Dicyclopentadiene	Caribe Isoprene Corp.	Ponce, PR
		Exxon Corp. Exxon Chem. Co., Div. Exxon Chem. Co., U.S.A.	Baton Rouge, LA
		Northwest Industries, Inc. Velsicol Chem. Corp., subsid.	Marshall, IL
		Union Carbide Corp. Chems. and Plastics Div.	Seadrift, TX
15.	Aldrin	Shell Chemical Co. Agricultural and Related Products	Denver, CO*
16.	Chlordane	Northwest Indust., Inc. Velsicol Chem. Corp., subsid.	Marshall, IL
		Prentiss Drug and Chem. Co., Inc.	Newark, NJ
17.	Dieldrin	Shell Chemical Co. Agricultural and Related Products	Denver, CO*
18.	Endrin	Northwest Indust., Inc. Velsicol Chem. Corp., subsid.	Memphis, TN

Table A.D-2 (Continued)

	Chemical	Company	Plant Location
19.	Chromium as Chromic Acid	Allied Chem. Corp. Indust. Chems. Div.	Baltimore, MD
		Chemetron Corp. Chems. Group Inorganic Chems. Div.	Cleveland, OH
		Diamond Shamrock Corp. Diamond Shamrock Chem. Co. Soda Products Div.	Castle Haynes, NC
		Essex Chem. Corp. Chems. Div.	Kearny, NJ
20.	Cadmium	The reader should refer to the 1973 Minerals Yearbook to obtain his own interpretation of this metal's mining status.	
21.	Heptachlor	Northwest Indust., Inc. Velsicol Chem. Corp., subsid.	Memphis, TN
22.	Nudrin (Methomyl) (Lannate^{R})	E.I. du Pont de Nemours and Co., Inc. Biochems. Dept.	La Porte, TX
		Shell Chemical Co. Agricultural Div.	Denver, CO
23.	Azodrin	Shell Chemical Co. Agricultural and Related Products	Denver, CO
24.	Bidrin	Shell Chemical Co. Agricultural and Related Products	Denver, CO
25.	Ciodrin	Shell Chemical Co. Agricultural and Related Products	Denver, CO
26.	Phosdrin (Mevinphos)	Shell Chemical Co. Agricultural Div.	Denver, CO

Table A.D-2 (Continued)

	Chemical	Company	Plant Location
27.	Nemagon (1,2-Dibromo-3-chloropropane)	Dow Chem. U.S.A.	Midland, MI
		Shell Chemical Co. Agricultural Div.	Denver, CO
28.	Hexachlorocyclopentadiene	Northwest Indust., Inc. Velsicol Chem. Corp., subsid.	Memphis, TN
		Occidental Petroleum Corp. Hooker Chem. Corp., subsid. Electrochemical and Specialties Div.	Montague, MI Niagara Falls, NY
29.	Methyl acetoacetate	Eastman Kodak Co. Eastman Chem. Products, Inc., subsid. Tennessee Eastman Co., Div.	Kingsport, TN
30.	Trimethyl phosphite	Mobil Oil Corp. Mobil Chem. Co., Div. Indust. Chems. Div.	Charleston, SC
		Occidental Petroleum Corp. Hooker Chem. Corp., subsid. Electrochemical and Specialties Div.	Niagara Falls, NY
		Stauffer Chem. Co. Agricultural Chem. Div. Specialty Chem. Div.	Cold Creek, AL Cold Creek, AL
31.	Allyl chloride	Dow Chem. U.S.A.	Freeport, TX
		Shell Chemical Co. Indust. Chems. Div.	Deer Park, TX
32.	Allyl alcohol	FMC Corp. Organic Chems. Div.	Bayport, TX
		Olin Corp. Designed Products Div.	Brandenburg, KY
		Shell Chem. Co. Indust. Chems. Div.	Deer Park, TX

Table A.D-2 (Continued)

Chemical	Company	Plant Location
33. Sodium chlorate	Brunswick Pulp and Paper Co. Brunswick Chem. Co., subsid.	Brunswick, GA
	Georgia-Pacific Corp. Chem. Div.	Bellingham, WA
	Kerr-McGee Corp. Kerr-McGee Chem. Corp., subsid.	Hamilton, MS Henderson, NV
	Occidental Petroleum Corp. Hooker Chem. Corp., subsid. Electrochemical and Specialties Div.	Columbus, MS Niagara Falls, NY
	Pacific Engineering and Production Co. of Nevada	Henderson, NV
	Penn-Olin Chem. Co.	Calvert City, KY
	Pennwalt Corp. Chem. Div.	Portland, OR Wyandotte, MI*
	Riegel Paper Corp.	Naheola, AL Riegelwood, NC
34. Calcium chlorate	City Chem. Corp.	Jersey City, NJ
35. Potassium chlorate	Kerr-McGee Corp. Kerr-McGee Chem. Corp., subsid.	Henderson, NV*
	Mallinckrodt Chem. Works Indust. Chems. Div.	Jersey City, NJ
	Occidental Petroleum Corp. Hooker Chem. Corp., subsid. Electrochemical and Specialties Div.	Niagara Falls, NY
	Pennwalt Corp. Chem. Div.	Portland, OR Wyandotte, MI*

Table A.D-2 (Continued)

Chemical		Company	Plant Location
36. Arsenic trioxide		Allied Chem. Corp. Specialty Chems. Div.	Marcus Hook, PA*
		American Smelting and Refining Co.	Tacoma, WA
		Apache Chems. Inc.	Rockford, IL
37. Arsenic trichloride		Allied Chem. Corp. Specialty Chem. Div.	Marcus Hook, PA*
38. Mercuric oxide	Red:	Mallinckrodt Chem. Works Indust. Chems. Div.	Jersey City, NJ
		Merck and Co., Inc. Merck Chem. Div.	Hawthorne, NJ
		Richardson-Merrell, Inc. J.T. Baker Chem. Co., subsid.	Phillipsburg, NJ
		Ventron Corp. Chems. Div.	Wood Ridge, NJ
	Yellow:	Mallinckrodt Chem. Works Indust. Chems. Div.	Jersey City, NJ
		Merck and Co., Inc. Merck Chem. Div.	Hawthorne, NJ
		Richardson-Merrell, Inc. J.T. Baker Chem. Co., subsid.	Phillipsburg, NJ
		Tenneco Inc. Tenneco Chems., Inc. Intermediates Div.	Elizabeth, NJ Long Beach, CA
		Troy Chem. Corp.	Newark, NJ
		Ventron Corp. Chems. Div.	Wood Ridge, NJ

Table A.D-2 (Continued)

Chemical	Company	Plant Location
39. Mercuric chloride	Mallinckrodt Chem. Works Indust. Chems. Div.	Jersey City, NJ
	Merck and Co., Inc. Merck Chem. Div.	Hawthorne, NJ
	Ventron Corp. Chems. Div.	Wood Ridge, NJ
40. Cuprous chloride	Allied Chem. Corp. Specialty Chems. Div.	Marcus Hook, PA*
	Chemetron Corp. Chems. Group Inorganic Chems. Div.	Cleveland, OH
	Diamond Shamrock Corp. Diamond Shamrock Chem. Co. Chemetals Div.	Curtis Bay, MD
	Filo Color and Chem. Corp.	Newark, NJ*
	Kerr-McGee Corp. Kerr-McGee Chem. Corp., subsid.	Powder Springs, GA
	Mallinckrodt Chem. Works Indust. Chems. Div.	St. Louis, MO
	Millmaster Onyx Corp. Millmaster Chem. Co., Div. Berkeley Chem. Dept.	Berkeley Heights, NJ*
	Southern California Chem. Co., Inc.	Chicago, IL* Garland, TX Metuchen, NJ* Santa Fe Springs, CA

Table A.D-2 (Concluded)

Chemical	Company	Plant Location
41. Nitrodiphenylamine		
2-Nitrodiphenylamine	American Cyanamid Co. Organic Chems. Div.	Marietta, OH
	Hummel Chem. Co., Inc.	South Plainfield, NJ*
4-Nitrodiphenylamine	Monsanto Co. Monsanto Indust. Chems. Co.	Sauget, IL
42. Hexamine (Hexamethylenetetramine)	Borden Inc. Borden Chem. Div. Adhesives and Chems. Div.	Demopolis, AL Fayetteville, NC
	E.I. du Pont de Nemours and Co., Inc. Biochems, Dept.	Belle, WV*
	W.R. Grace and Co. Indust. Chems. Group Dewey and Almy Chem. Div.	Nashua, NH
	Occidental Petroleum Corp. Hooker Chem. Corp., subsid. Durez-Stevens Div.	North Tonawanda, NY
	Plastics Engineering Co.	Sheboygan, WI
	Tenneco Inc. Tenneco Chems., Inc. Intermediates Div.	Fords, NJ
	Union Carbide Corp. Chems. and Plastics Div.	Bound Brook, NJ
	Wright Chem. Corp.	Acme, NC

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*This plant is no longer in operation.

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