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FINAL DRAFT REPORT

AN INTEGRATED GEOGRAPHIC APPROACH TO DEVELOPING TOXIC SUBSTANCE CONTROL STRATEGIES

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1. INTRODUCTION

1.1 BACKGROUND

The Environmental Protection Agency, through its Toxics Integration Program, is currently investigating a number of alternative regulatory approaches for dealing with toxic substances in the environment. Pilot projects have been conducted to examine the feasibility of regulating toxic pollutants on an industry-by-industry, chemical-by-chemical, or geographic basis. The goal of these projects is to develop feasible and cost-effective regulatory approaches that will rectify specific environmental problems while minimizing the economic burdens of compliance. By addressing multi-media environmental issues in an integrated fashion, it may be possible to manage toxics exposure problems in a more efficient manner than the traditional "command and control" approach which separately addresses each medium.

This report presents a preliminary framework for the geographic approach to development of toxics control strategies. It represents a general methodology which was developed in conjunction with a pilot study of the Kanawha River Valley in West Virginia. Details of the pilot study are presented in a separate report.* The underlying concept of the geographic approach is that control strategies can be developed on a site-specific or region-specific basis, possibly with assistance from state and local governments and other groups, such as industry associations. To pursue this type of approach, the EPA would require a site selection procedure for identifying candidate geographic areas with significant potential for environmental toxics problems. The feasibility of such a procedure is currently being investigated by the EPA, but is not included in the scope of this report. Thus, the general methodology described here will assume that a specific study area has already been designated.

*"An Integrated Geographic Study of Potential Toxic Substance Control Strategies in the Kanawha River Valley, West Virginia", Arthur D. Little, Inc., Final Draft, August 31, 1981.

The concept of a geographic approach is not new to the EPA; several earlier studies have attempted to assess the impact of toxic substances in specific local areas and to investigate the need for controls. For example:

- The EPA performed a study in 1978 to evaluate the levels of pollutants in air and water for the Beaumont, Texas/Lake Charles, Louisiana area, with emphasis on collection of monitoring data.

- EPA Region IV organized a geographic study of toxic substance sources and pathways for the Memphis, Tennessee area in 1980, partially in response to public complaints of pollution from waste dump sites. The same Region is currently initiating a carefully-planned study of the Louisville, Kentucky area, with participation from governmental and citizen groups.

A good deal of useful information was obtained from these previous studies, although it is not the intent of this report to review them in detail. The present geographic methodology builds upon these experiences, but is unique in that it addresses multiple chemicals, sources, pathways, and receptors within a unified technical framework. The methodology is designed to be predictive, in the sense that it identifies potentially significant pathways from pollutant sources to receptors, and allows quantitative evaluation of the cost/benefit tradeoffs of alternate control strategies that seek to reduce these exposures. The integrative multi-media approach ensures that control of a pathway in one medium does not overlook the potential displacement of toxic substances into other media which are not sufficiently controlled. By focusing upon a specific geographic area, the EPA can achieve a richness of descriptive detail that is not possible with a broader national scope of investigation, and will encourage appropriate local solutions to local problems.

1.2 OBJECTIVES OF THE GEOGRAPHIC APPROACH

The geographic approach to regulation of toxics in the environment provides an alternative to regulatory programs based on national or industry-specific considerations. Under the geographic approach a selected local area would be examined as a whole for potential environmental problems. The investigation would include all sources of toxics in the area and all possible routes of exposure for humans and other biota. If problems are detected, control strategies would then be devised to mitigate these problems in an efficient manner. The objectives of the geographic approach may be stated as follows:

- To select a small number of sites across the U.S. which appear to have the greatest likelihood of environmental toxics problems.

- For each specific site, to select toxic substances of concern, to evaluate their sources, inter-media pathways, and population exposures, and thus to identify any existing or potential problems.

- For each toxics problem designated, to evaluate the feasibility, the costs, and the benefits of alternate control strategies, which may exploit either Federal, State, or local authorities.

- To provide a comprehensive data base and analytic capability for ongoing environmental surveillance and protection in the study area.

The scope of the present methodology is limited to analysis of exposures to toxic substances, without explicit quantification of health effects. Also, attention is confined to exposure arising due to the presence of toxics in the ambient environment; occupational and consumer use-related exposures are <u>not</u> addressed. These are not inherent limitations to the geographic approach, but reflect the current emphasis of the EPA Toxics Integration Program. Further discussion of these limitations in scope is provided in Section 8.2.3.

1.3 SITE SELECTION REQUIREMENTS

In order for a geographic approach to be implemented on a regular basis, certain realignments would be required in the conduct of EPA's existing programs and in the allocation of resources. Due to the intensive technical and data reauirements of a geographic study, no more than a few such studies could be in progress during any given period of time within a Region. This implies the need for a priority-setting mechanism; that is, a site selection procedure that would identify likely candidates for geographic areas to be studied in detail. It will be important to ensure that this procedure is applied in a consistent and unbiased fashion across different regions. Criteria for site selection would probably include the following factors:

- Significant toxic levels in the ambient environment
- Presence of numerous potential sources of toxics (including abandoned sites)
- Proximity of substantial population groups to toxics sources
- Evidence of health effects or environmental damage

The development of a site selection procedure is a complex undertaking due to the multiplicity of pollutants, source categories, and environmental scenarios that must be considered. It is expected that the procedure will involve several iterations, incorporating both subjective assessments and computerized ranking methods to arrive at a final list of sites. The States will no doubt play a leading role in this process, and it will also be important to utilize the EPA Regions' intimate knowledge of each specific area within their authority. The site selection procedure would have to be flexible enough to accept a wide variety of inputs, yet sufficiently well-defined that it could be repeated whenever additional sites need to be selected. A preliminary outline of such a procedure has already been developed under to Toxics Integration Program, and its feasibility is being explored.

1.4 SUMMARY OF METHODOLOGY

1.4.1 Overview of Geographic Study

The technical methodology for conduct of the geographic study is the central concern of this report, and is described at length in the remaining chapters. There are three major phases in the approach proposed here, and they are depicted in simplified terms in Figure 1-1. These three phases are summarized individually below:

Phase 1: Data acquisition, study boundary definition, initial scan of significant enviornmental pathways, and selection of pollutants. (This phase is described in Chapter 2.)

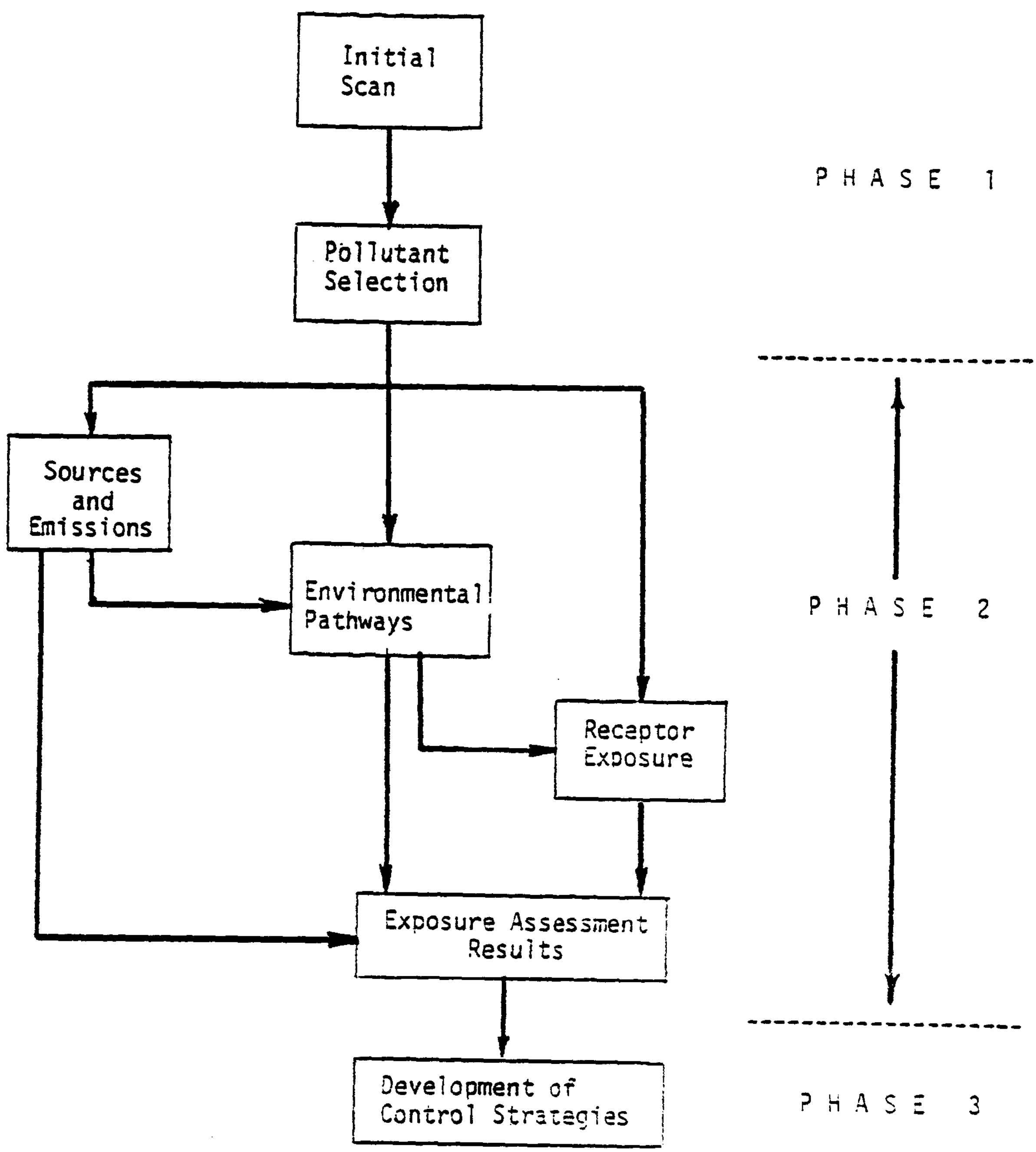
Phase 2: Detailed exposure assessment, including quantification of source emissions, modelling of chemical fate and transport pathways, and quantification of receptor exposure routes in various media. (This phase is described in Chapters 3, 4, 5, and 6.)

Phase 3: Identification of potential toxic substance problems, collection of additional data, and evaluation of costs and benefits of alternate control strategies. (This phase is described in Chapter 7.)

The purpose of Phase 1 is to set priorities and lay the foundation for the more detailed work in Phase 2. The outcome of the second phase is a description and quantification (where possible) of potential exposure levels by pollutant and receptor category. Moreover, the origins of these exposures can frequently be traced back to the probable pollutant sources by means of the environmental pathways analysis. At this juncture certain problem areas may be identified that are due to excessive environmental loadings or ambient levels. Several different courses of action are possible in Phase 3:

FIGURE 1-1

FLOW DIAGRAM FOR GEOGRAPHIC STUDY



- Where clear violations of existing standards or regulations have been detected, enforcement actions may be initiated.

- Where potential problems are suggested by the exposure assessment, additional data (e.g., field sampling or health effects data) may be collected to verify these findings.

- Where potential problems are of sufficient gravity, the Centers for Disease Control (CDC) may be consulted regarding the development of a public health protection plan for imminent hazards.

- Where the possibility of long-term human health effects is suggested, epidemiological studies may be initiated for specific pollutants; the CDC can also be helpful in this regard.

- For those problems not requiring immediate action, and for which sufficient data are available, consideration can be given to the relative advantages of different control strategies.

This last step will be the focus of the Phase 3 methodology described in Chapter 7. There will in general be a large array of control options available to address a specific toxic substance problem, depending upon the nature of the problem and the degree to which sources can be identified. State and local control options as well as Federal ones have been considered, and a framework for selecting cost-effective strategies is presented. However, due to the immense variety of situations that may be encountered, the methodology is best understood by means of the Kanawha Valley pilot study example. (See footnote on page 1-1.)

Finally, once a geographic area has been thoroughly studied and the necessary controls implemented, the study report would provide a comprehensive basis for ongoing surveillance and revision of control strategies. It would be the responsibility of the EPA Regional Office to maintain cognizance of changes in the relevant source configuration, receptor distribution, or environmental conditions, and to coordinate with State or local agencies in responding to these changes as necessary. Chemical inventories, pathway models, and population exposure indices developed in the course of the geographic study could be maintained and updated periodically with a low level of effort, thus providing appropriate tools for ensuring that adequate toxics controls are maintained in the future. Many of the normal Regional activities could be adapted to coordinate with this evolving geographic "profile", so that redundancy in collection or interpretation of data would be minimized. In this way, the study would not become obsolete, but would remain a useful and pragmatic instrument for carrying out EPA policy.

1.4.2 Exposure Assessment Approach

The exposure assessement portion of a geographic study constitutes the second Phase, as defined above. During this phase, a detailed quantification is performed of the sources, pathways, and receptor exposures for the toxic substances selected during Phase 1. A large part of the data required for the exposure assessment will have been gathered during the first Phase, so that the exposure assessment work will involve mainly analytic efforts and computer modelling. However, additional data collection may be necessary for specific inputs to various tasks, such as meteorological information for the air pahtways analysis or population data. An overview of the methodology is presented here, and then Chapters 3 through 6 describe each of the individual tasks.

In Phase 2, for those pathways and chemicals considered important as a result of the initial scan, a more detailed data analysis is performed. The analysis is guided by the pentagram framework shown in Chapter 2, Figure 2-1. Five separate tasks are performed, roughly corresponding to the five matrices shown in the pentagram framework. Starting from the pollutant axis, these five tasks can be traced by moving counter-clockwise within the framework. Figure 1-2 shows the flow of information among these tasks.

- Task 1--Identification of Pollutant Sources (see Chapter 3)

  For the list of pollutants being considered, an inventory is performed of the various categories of sources, including industrial, commercial, residential, and other sources where these pollutants may be produced, used or found as by-products.

- Task 2 -- Quantification of Emissions (see Chapter 3)

  The environmental emissions or discharges from each of the source categories and for each of the pollutants considered is quantified, where possible. In this way the total environmental loading of pollutant emissions is established for each of the receiving media considered.

- Task 3 -- Environmental Pathways (see Chapter 4)

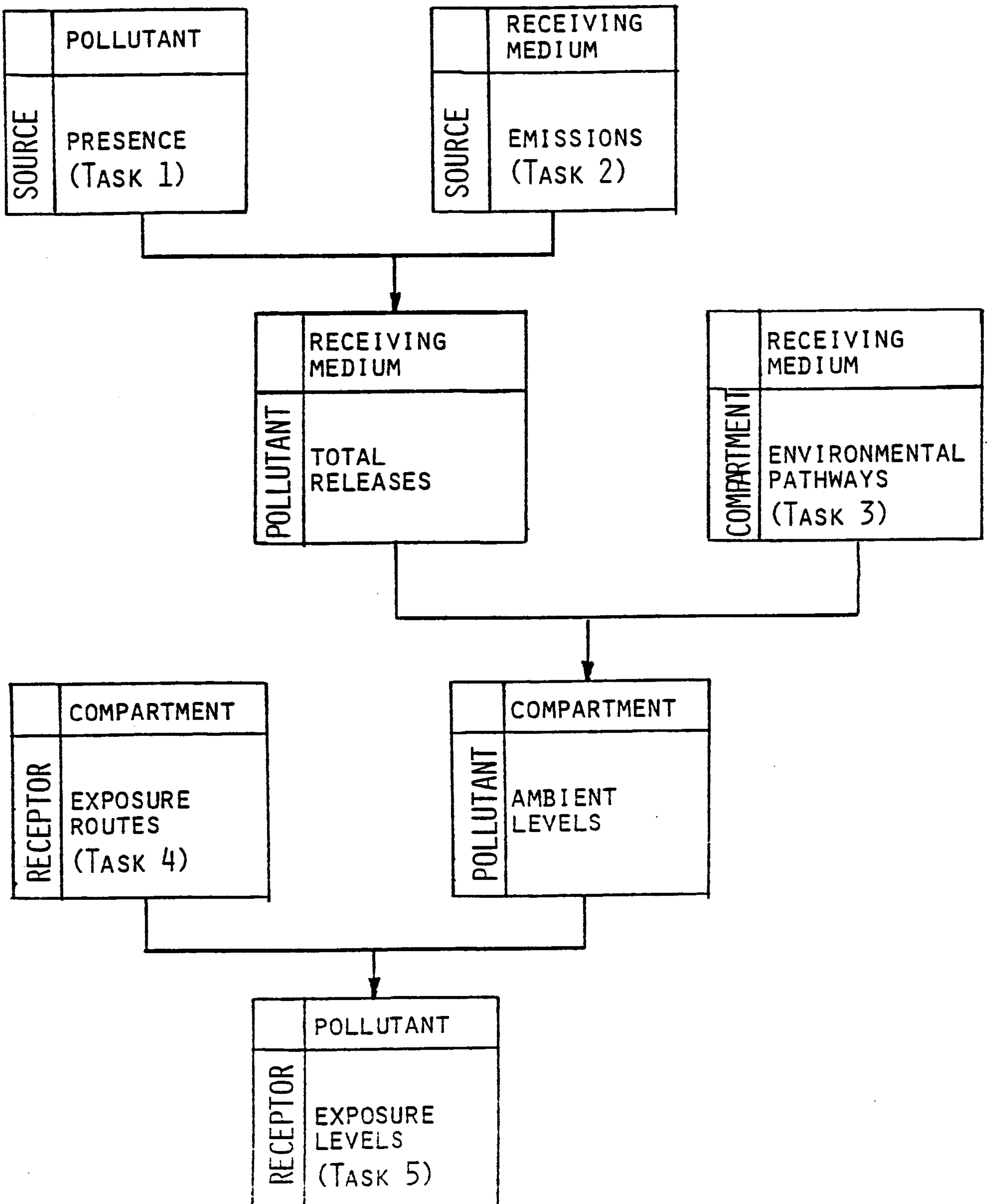
  For a selected number of pollutants that are discharged into the various receiving media, their fate and transport in the environment is investigated through modelling, monitoring data or other means. As a result, the environmental levels of these pollutants are estimated, where possible, for ambient air, surface water, drinking water, biota, and other environmental compartments that are pertinent to receptor exposure.

- Task 4 -- Receptor Exposure Routes (see Chapter 5)

  For each of the receptor categories of concern, including humans, aquatic organisms or other organisms in the food chain, their exposure to the various environmental compartments addressed in the previous task is quantified, where possible. Exposure is expressed in terms of the extent and

FIGURE 1-2

FLOW OF INFORMATION FOR EXPOSURE ASSESSMENT



frequency of contact with the environmental compartments discussed above through inhalation, ingestion and absorption.

- Task 5 -- Exposure Assessment (see Chapter 6)

  As a result of the previous four tasks exposure pathways are established between sources and receptors. The final task is concerned with estimating, where possible, the quantity or concentration of each pollutant to which the various receptor categories may be exposed.

1.5. INCORPORATION OF HEALTH EFFECTS DATA

Although the exposure assessment described above can be revealing in terms of specific population exposures to toxic emissions, it may be argued that the final criterion for control strategy selection should be related to health effects rather than exposure. Since different substances may have different effects and different levels of potency, the health impacts of exposure to these substances may vary considerably. In particular, it is possible to compare the potential long-term effects of various substances in rough quantative terms, using the dose/response extrapolation techniques that were adopted by EPA's Carcinogen Assessment Group. In this way, the reduction in exposure that might be achieved by a particular control strategy can be evaluated in terms of the corresponding risk reduction that is predicted for the exposed population. Such a risk assessment can provide the appropriate common denominator for balancing exposures to different substances in different environmental media.

When incorporating health effects data, it is important to note the limited accuracy of available risk estimation techniques. For example, the following qualifications must be kept in mind when utilizing carcinogenic risk estimates:

- The human carcinogenicity of most substances is not established, and species differences may exist between human responses and those of laboratory animals.

- Estimation of equivalent human doses requires the use of scaling factors whose accuracy is open to question.

- The shape of the dose/response curve at low doses is unknown, and different dose/response models can yield widely differing results.

Assuming that laboratory data can indeed be applied to humans, and assuming a particular dose/response relationship, exposure assessment results can be used to predict the potential incidence of cancer in an exposed population. Though there may be considerable uncertainty in such predictions, they can serve as a useful guide to problem identification and policy formulation.

1.6 ADMINISTRATIVE ISSUES

The purpose of this report is to present an appropriate technical methodology for performance of a geographic study. It is important to note, however, that for a geographic study to be successfully implemented, it is essential that a suitable management plan be developed for carrying out the technical work. Due to the complexity of the multi-media approach and the potential concern of state and local interest groups, a considerable amount of planning and coordination will be necessary before launching a geographic study in a particular area. Some of the main issues that need to be resolved include:

- Authority and approval--the responsible agencies for performance of the study must be identified, and approval must be obtained from any groups (such as local governments) that may be affected by the conduct or findings of the study. In particular, clearance must be obtained, if necessary, for use of restricted data.

- Technical resources--the participants in the study, both managerial and technical must be identified, and sources of funding must be established. Due to the complexity and sensitive nature of a geographic study, it will be advisable to form a study team that draws upon Federal, State, and local resources. This approach may facilitate the acquisition of site-specific data, such as local agency records and files.

- Public information--when a geographic study is initiated, local governments, industries, and the general public will have to be notified of the study. From a public relations point of view, it is important that the EPA clearly articulate the goals of the study - namely, to ensure the continuing protection of public and environmental health. Rumors or misunderstandings may create false beliefs about the existence of imminent hazards, which will serve only to obstruct the conduct of a rational, scientific study. Therefore, the initial planning and organization of the study is crucial to its ultimate success and credibility.

Though it is not the intent of this report to address these administrative issues, they will be no less important than methodological issues in the implementation of a geographic approach. Adoption of this approach as an ongoing EPA program could fundamentally alter the Agency's allocation of resources and institutional practices. Therefore the potential benefits and obstacles associated with this approach need to be carefully examined.

2. PRELIMINARY PROCEDURES

2.1 INTRODUCTION

This section describes the procedures that are necessary during Phase 1 of a geographic study. The purpose of Phase 1 is first to define a geographic boundary for the study, and then to develop a rapid understanding of the potential environmental problems within the geographic area by scanning the available data concerning emissions, ambient levels, and exposures. Relevant data must be collected and interpreted in order to determine what the significant exposure pathways might be, and to identify any data gaps that need to be resolved. The framework for this phase is provided by the pentagram structure shown in Figure 2-1. This framework allowed simultaneous consideration of pollutants, source categories, receiving media, environmental compartments, and receptor categories in order to identify potentially important pathways of exposure. This framework also provides the basis for the detailed exposure analysis performed in Phase 2. For the purposes of initial scanning, a qualitative identification is made of pollutants within source categories, of emissions from source categories to receiving media, of the fate of pollutants within the various environmental compartments of concern, and of the exposure of various receptors to these environmental compartments. Those chemicals and pathways which are considered most significant on the basis of the available data will then be subjected to more careful scrutiny in Phase 2.

An important issue during Phase 1 is the availability of data for the various analytic tasks of Phase 2. For most geographic areas there will be significant data gaps that will limit the completeness and accuracy of the exposure assessment. Data requirements and potential data sources are discussed in Section 2.4, but the available data will most likely have to be supplemented by a program of new data acquisition. It is anticipated that new data will be required in one or more of the following categories:

- Emission rates or environmental loadings of major point and non-point sources for air, surface water, or land disposal.

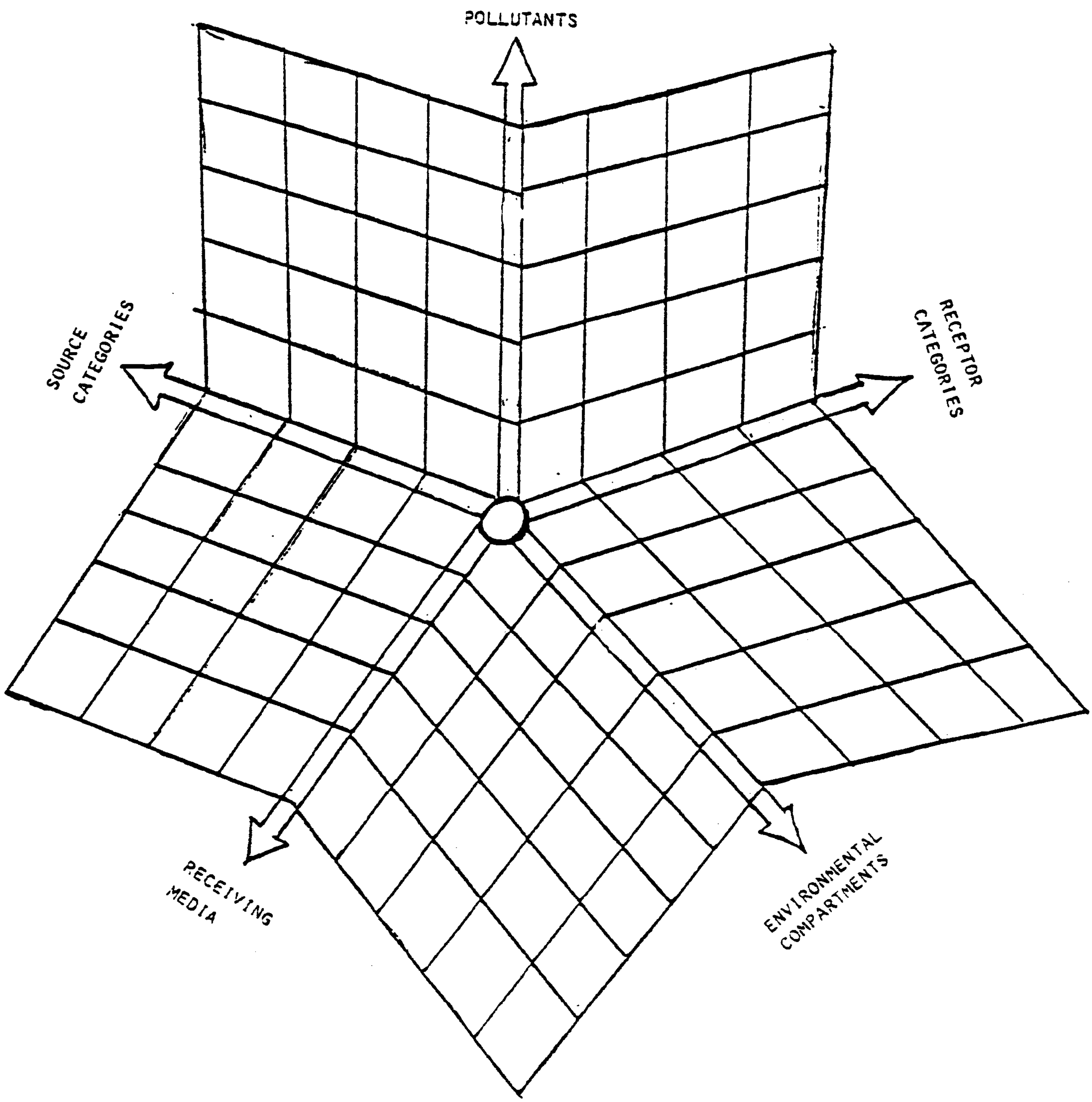


FIGURE 2-1

PENTAGRAM FRAMEWORK FOR A GEOGRAPHIC STUDY

- Ambient concentrations of selected toxics in air, surface water, groundwater, drinking water, sediment, or soil for different seasons of the year.

- Concentrations of toxics in fish or animal tissue, in food, in crops, and possibly in human tissue.

Thus a significant field sampling effort may be necessary during the course of a geographic study, in order to assemble an adequate data base. Though a long time period would be required to capture seasonal variations, the sampling program could be conducted in parallel with the exposure assessment. In fact, findings about potential high exposure scenarios could influence the choice of sampling locations, and conversely the discovery of unusual toxics levels could alter the focus of the exposure assessment. The detailed design of such a sampling program would depend upon site-specific circumstances, and therefore is not addressed in this report. However, guidelines for the data requirements are presented in Section 2.4 and in the subsequent Chapters. An efficient means of acquiring field data might be to incorporate the study area within one of the national monitoring programs conducted routinely by EPA, FDA or other agencies.

2.2 STUDY BOUNDARY DEFINITION

After a problem area has been selected for a geographic toxics study, the study area boundaries must be delineated in order to allow for a systematic analysis. The proper selection of study boundaries is critical to the entire geographic study because the sources of toxics and exposed populations that are included in the study area will directly affect the findings. Study boundary delineation requires intuitive as well as objective judgment, because the information that would be useful is often not available until after the boundaries have been tentatively selected. Study boundaries will generally need to be modified for the different phases of the exposure analysis and control strategies development because of differences in the nature and goals of each phase. In practice, the study boundaries determined initially may be modified later in the study as more information becomes available. A tentative emissions inventory study area will be defined prior to the initial scan, based on available information. These boundaries may be modified on the basis of information collected in the initial scan, and may again be changed to incorporate sources of toxics discovered later in the data collection and analysis. The study areas for the environmental pathway analysis and the exposure assessment will depend on the results of the emissions inventory. Similarly, the area considered for control strategies will depend on the results of the other analyses. The important factors to consider when selecting study area boundaries are presented below for each of the major phases of a geographic toxics study.

Sources and Emissions Inventory

The objective in delineating a study boundary for the inventory of sources and emissions of toxics is to encompass all areas containing sources of toxics while excluding areas that are not potential sources within the general area designated for study. In the ideal situation, the study area would consist of a geographic area in which toxics produced are self-contained and which receives no significant imports of toxics from locations outside the study area boundaries. This situation is rare, however; in practice, imports and exports of toxics must be estimated or assumed negligible.

A tentative study area boundary, delineated prior to the initial scan, will depend on the information available to the investigators at the start of the study. If the area was designated a problem area on the basis of known sources of toxics (e.g., industries, waste disposal sites), the tentative boundaries will be determined on the basis of locations of the potential sources. If, on the other hand, the bases for concern are ambient or epidemiological data suggesting toxics of unknown origin, consider the transport modes of the toxics in order to include all potential sources of toxics within the study area boundaries. During the initial scan, toxics data for the entire tentative study area must be sought, as well as other relevant data that might be the basis for modification of the study area boundaries. Using the data collected in the initial scan, refine the study area boundaries, if necessary, to better suit the needs of the study.

In order to maximize accuracy and efficiency, physical factors that affect the collection or analysis of data must be considered in delineating study area boundaries. For instance, if preliminary data suggest that non-point source runoff is a significant source of toxics in the study area, the emissions inventory study area boundaries may have to be defined by subwatershed, because non-point source pollutant loads are most accurately estimated on a subwatershed basis, whereas other source/emission analyses may be flexible. Similarly, if perusal of the initial ambient data suggests that a number of undeveloped subwatersheds are not significant toxics sources, delete these subwatersheds from the study area in order to save time and effort. In addition to physical factors, anthropogenic factors must be considered in the delineation of the source and emissions study area; in cases where there are significant imports of toxics via natural (e.g., air, surface water, groundwater) or man-related (e.g., truck, train) transport, the geographic area for which data must be collected will be larger than the designated study area.

Consider political and socioeconomic factors when selecting study area boundaries for the emissions inventory, but only after practical and scientific requirements have been met. The aforementioned physical factors that affect data collection and analysis, and the actual distribution of potential sources of toxics are more important than political and socio-economic factors, because toxics problems are rarely restricted to one city, township, or county. In the cases where a political boundary meets the scientific needs of the study, however, the use of this boundary may facilitate data collection and analysis. For example, if the study area boundary coincides with a county boundary, the researchers can save time and effort by not collecting data on the excluded county.

Environmental Pathway Analysis

The study area for the environmental pathway analysis will depend on the areas designated for the emissions inventory and the exposure assessment. The boundaries for this analysis are determined based on consideration of the results of the emissions inventory, the initial scan of environmental data (geological, topographical, meteorological, hydrological), monitoring data, and population data. The emissions inventory will indicate the areal extent of sources of toxics. Use the environmental data in conjunction with the demographic data to make general projections of the areal distributions of the populations of interest that might be exposed to the identified sources of toxics. Ambient monitoring data, if available, are particularly helpful in determining study boundaries because they provide direct information on the environmental pathways of toxics from the sources. Because the purpose of the environmental pathway analysis is to trace the movement of toxics from source to receptor populations, the modeled study area must encompass both the emissions inventory study area and the population exposure study area (discussed below).

Exposure Assessment

The appropriate study area boundary for the assessment of exposure in a geographic study will not necessarily coincide with the study area for the emissions inventory. The objective in delineating the exposure study area is to include all areas containing populations potentially affected by toxics, while excluding from consideration the unexposed populations. To some extent, the study area for the exposed population will be dictated by the history of the particular study. If epidemiological data suggested a toxics problem in a certain population, then the study area is best defined on the basis of the geographic location of that population (e.g., a city and its suburbs). Alternatively, if the toxics study was initiated because of the existence of a number of potential sources of toxics in the general area, the boundaries for the exposure assessment will be delineated only after the emissions inventory has been completed and the data relating to transport of toxics have been examined. As stated previously, tentative study boundaries for the exposure assessment will be determined prior to the environmental pathway analysis, because the pathway analysis study area depends on the areal extent of populations that are expected to be exposed to toxics. The use of available monitoring data is recommended, because these data indicate areas where toxics exposure may occur. It is recommended that the exposure study area be modified if the environmental pathway analysis suggests that the exposure of some populations in the tentative study area is negligible and/or the exposure of the populations not included in the tentative study area is significant. For example, if the modeling suggests that toxic concentrations in ambient air are high in a residential area previously thought to be unaffected by a distant source, expand the study area to encompass that residential area. Likewise, if the modeling predicts that toxic concentrations are negligible in a recreational lake that was included in the tentative exposure assessment study area boundary, the lake can be omitted from any further consideration with regard to exposure in order to save time and human resources.

In practice, the optimal study area for analysis of population exposure may be highly irregular, and may in some cases be represented by a central area and several satellite areas. For instance, a town outside the main boundaries of a study area will be included as a "satellite" to the main study area if its drinking water is obtained from a source within the main study area. In the hypothetical case concerning a highly industrialized area adjacent to a river, the available data on toxics emissions and environmental transport may dictate that the exposure study area include a long narrow segment of river and adjacent floodplain downstream of the industrial sources. Boundaries may also be refined to be made compatible with census bureau delineations. It should be noted that, in some cases, human or wildlife populations that are not permanent residents of a study area must be included in exposure analysis; population and activity data for commuters, vacationers, and migratory animals will have to be estimated from data other than local census bureau statistics.

In some cases, it may be worthwhile to consider the existing political boundaries in delineating study area boundaries for exposure analysis. As in the case of emissions inventory study area boundaries, however, use municipal, county, or state boundaries only if they satisfy the technical needs of the study. Consider political boundaries in delineating the study area boundary in cases where the available census data correspond to these boundaries.

Control Strategies

The study area boundaries for the development of control strategies will generally encompass the geographic areas considered in the analysis of emissions, fates, and population exposure and will depend on the results of these analyses. Because the implementation of some control strategies will depend on local, regional, and national political and socioeconomic factors, the effective study area may correspond to municipalities, counties, or states in which the toxics problem is located. Thus, the geographic area to consider in the development of control strategies may be as small as the areal extent of toxics sources and affected populations or as large as a state or a region.

2.3 DATA ACQUISITION

Data acquisition begins as soon as the toxics integration study is underway. This subtask is crucial to the entire geographic study, because the acquired data are the foundation for all subsequent analyses. It is also the limiting factor for progress in other preliminary procedures, because the delineation of study boundary, pollution selection, and the initial scan are all dependent upon the available data base. Ideally, most of the data are acquired prior to the initiation of Phase 2 (detailed exposure assessment). In practice, however, data acquisition is an ongoing process and "late" data must be incorporated into the study whenever it arrives.

The goal of the data acquisition subtask is to identify and acquire all available information relevant to toxics sources and emissions, environmental pathways, exposure, and toxics control in the study area. To fulfill this goal, considerable general background information is necessary in addition to data specifically related to toxics. For example, information on the geology, hydrology, soils, meteorology, demography, and regulations pertaining to the area is vital to the analysis of toxics problems and the development of control strategies. It is recommended that site-specific data be used wherever possible in the geographic study, because these data are generally most accurate. When site-specific data are not available, however, surrogate (i.e., regional or national) data must be acquired.

Because the data acquisition subtask is concurrent with the selection of pollutants, the list of toxics to be considered in the study may not be finalized until some of the acquired data have been examined. Therefore, information relating to all possible toxics candidates must be sought until the final pollutant list is known; thereafter, data acquisition should concentrate exclusively on the toxics selected for the study. For the selected toxics, it is crucial that the investigators familiarize themselves with general published information on the production, use, emissions, environmental fate, and environmental and health effects in the early stages of data acquisition. With this information, compile a list of all possible sources (e.g., industry, commercial)/discharge modes (e.g., point source water, solid wastes) for each toxic. During the course of data acquisition, investigate each potential source/discharge mode with respect to the study area.

Most of the toxics information will be available through various government agencies. Because the specific agencies responsible for collecting and compiling the data used in a geographic study of toxics vary from place to place, it is not possible to develop an exact "blueprint" to follow in the acquisition of data. It is recommended that investigators contact officials at the local, state, and federal level in order to determine which agencies can provide the necessary information. A general summary of the data requirements and data sources for each task of the geographic study is presented in Table 2-1. More detailed descriptions of the data needs and data sources for each phase are given in Chapters 3-7.

In all geographic studies there will be substantial gaps in the available site-specific data that must be filled by surrogate (regional or national) data. Even for areas where toxics have been relatively well studied there will be gaps in the information on some toxics sources, emission rates, environmental pathways, and exposure routes. While some of the information can be obtained by acquiring new data (e.g., conducting a monitoring program), this option is costly; consequently, surrogate data will often be used in geographic studies. For this reason, it is

Table 2-1. Summary of Data Requirements and Possible Sources of Data for a Geographic Toxics Study

Class of Data	Possible Sources of Data
Pollutant Sources and Emissions • Computerized surveys of chemical manufacturers. • Surveys of manufacturers and users. • Computerized monitoring data. • Emissions permits, registrations, data, and inventories. • Detailed land use information. • Generic information on sources and emission. • Demographic data.	Federal: EPA Headquarters (computerized data bases and technical reports) EPA Regional Offices (Air Quality Monitoring Branch, Water Quality Monitoring Branch, Hazardous Waste Task Force, Enforcement Branches, Environmental Emergency Branch (Surveillance and Analysis Division), Pesticides Branch. Also, U.S. EPA Water Quality Analysis Branch for NURP and POTW Studies and Effluent Guidelines Division. U.S. Army Engineer District U.S. Department of Agriculture (Geological Survey, Office of Surface Mining), River Basin Commissions State: department responsible for environmental affairs or natural resources, health department, office responsible for solid and/or hazardous wastes, office responsible for air pollution control, agriculture department, mining agencies Others: direct contact with sources local soil conservation district office; county, township, or municipal offices responsible for environmental affairs, natural resources, health, and solid waste; chambers of commerce; published literature
Environmental Fate • Climatic data: i.e., precipitation, wind direction, wind speed, temperature, pressure, etc. • Hydrologic data: i.e., surface and ground water distribution, quantity, etc. • Soil data: i.e., soil classification, geology, soil permeability, etc. • Land use data. • Chemical fate data: physical, chemical and biological properties of pollutants. • Monitoring data: concentrations of pollutants in environmental compartments.	Federal: National Weather Bureau, NOAA, USGS, USDA (Soil Conservation Service), U.S. EPA Water Quality Analysis Branch (STORET/TOXET data bases, REACH, stream gage data), EPA technical documents, Bureau of Mines. State: Departments responsible for environmental affairs or natural resources, departments responsible for geological and economic surveys, soil conservation department, air pollution control, water development authority Others: universities, county and city offices, published literature

Table 2-1. Summary of Data Requirements and Possible Sources of Data for a Geographic Toxics Study (continued)

Class of Data	Possible Sources of Data
Exposure Routes • Population data for humans broken down into regional distribution, sex and age classes, special groups. • Occupational statistics. • Data on food consumption patterns, sources of drinking water and populations supplied, recreational patterns. • Information on locations of areas with potentially high exposure (beaches, playgrounds, industries from previous tasks). • Use information for specific products important in terms of exposure. • Documentation of actual incidents of exposure. • Human tissue and other biological media monitoring surveys. • Health effects surveys. • Species and population surveys for fish and wildlife. • Surveys of natural plant species and agricultural statistics. • Endangered and threatened species lists - Federal and state.	Federal: Bureau of Census, Department of Agriculture, Department of Interior - other offices (endangered species, U.S. Fish and Wildlife, Bureau of Land Management), HEW (NIOSH, CDC, FDA Fish and Crop Monitoring), U.S. EPA Water Quality Analysis Branch (fish kills), TSCA substantial risk notices, USGS Water Quality Alert. Regional EPA: Environmental Emergency Branch, Water Development authority, Office of Special Programs, Exposure Evaluation Division State: departments responsible for natural resources (parks and recreation, water resources, wildlife resources), environmental health, community health services, geological and economic survey, agriculture. Others: state and local planning departments, local conservation groups (i.e., Audubon), universities, community health organizations, contact with manufacturers or local retailers, ADL Risk Assessment Methodology Report, past ADL risk assessments, other literature.
Control Strategies • Federal and state air emissions standards. • Federal and state water effluent standards and guidelines. • Federal and state hazardous and solid waste regulations. • Federal and state ambient air standards. • Federal and state ambient water standards. • OSHA standards. • Exposure criteria. • Technological control options.	Federal: EPA technical reports, Occupational Safety and Health Administration, Food and Drug Administration, Code of Federal Regulations and Federal Register State: code of regulations Others: universities, published literature, contact with generators of toxics

recommended that the EPA assemble generic data on sources, emissions, environmental pathways, and exposure routes in the event that the geographic approach to toxics control is adopted. Much of this information would be of use to the industry-by-industry and chemical-by-chemical toxics integration activities as well. If such surrogate data is easily accessible to personnel conducting geographic studies, the time spent tracking such information would be kept to a minimum. Furthermore, knowledgeable EPA personnel could assure quality control by selecting the "best" set of surrogate data from all available data for use in geographic studies.

Aerial Reconnaissance

The initial scan can be aided by the use of aerial reconnaissance and related photographic imagery. Several data sources covering different parts of the country at different times are available through the EROS Data Center in Sioux Falls, South Dakota, the U.S. Army Corps of Engineers and the U.S. Geological Survey. Photo-coverage of some areas may go back to 1945 and can be used to establish a historical imagery file for a selected site. Such a file can be used to identify abandoned pollution sources such as old dumps, landfills and areas of soil filling, industrial impoundments, tanks and tank farms, drum-related sites, auto junkyards and stacks.

The Environmental Photographic Interpretation Center (EPIC), a field station of EPA's Office of Research and Development and Environmental Monitoring Systems Laboratory, Las Vegas, has developed a computer-aided image interpretation capability. They have prepared many historical land-use maps using photographic imagery for various site-specific studies. Their approach is linked to USGS guidelines for Level I, II and III land-use categories, and permits the use of high resolution U-2 overflight imagery which is produced by NASA through an inter-agency agreement. Current overflight coverage through a U-2 flight can be obtained for an entire state at a fairly reasonable cost. The entire state of Pennsylvania was recently done in this regard and the State of West Virginia is a target for an overflight program some time in 1981.

The imagery data can be interpreted through microscopic and stereoscopic viewing of the imagery by persons expert in environmental, land-use, and imagery analysis. The information is extracted and transferred to overlaid map sheets, employing the USGS land-use codes. The resulting information for a single site can best be used as a comprehensive information base detailing overall development in and around an area. Specific pollution sources can be analyzed in relation to land-use changes over the period of time covered by the historical imagery. Long-term trends in land-use can be mapped and used to predict the presence of potential pollution sources due to changing land-use patterns. Such data collection technologies could be usefully employed in identifying the boundaries of a geographic study area and in confirming the presence of potential pollution sources not detectable through field observation (e.g., tanks behind a stand of tall trees on private land), or through national or state data bases.

2.4 POLLUTANT SELECTION

The number of toxics likely to be present within any one geographic area will probably be too many to allow individual consideration of each one in a regional study. Therefore, it is important to have an efficient and effective procedure for selecting the toxics that merit study. The procedure should be well-defined and reproducible so that it can be used at any location, but flexible enough to accept the variety of information needed to select the group of pollutants. This section is a discussion of a recommended approach for pollutant selection.

The objective of this approach is to identify a group of pollutants which meet at least one of the following criteria for a specific geographic area:

- the most significant direct or indirect releases of toxics in the geographic area including industrial, municipal, commercial, domestic and natural sources.
- evidence of substantial ambient levels in air, surface and ground water, or biota.
- potential for significant acute or chronic health problems to humans and other biota due to:
  - -- toxicity;
  - -- likelihood and degree of human and other biotic exposure via inhalation, ingestion of drinking water and food, dermal contact, etc.

The final list selected will reflect the characteristics of the geographic region under study. For example, in a heavily industrialized area, the pollutants chosen are likely to be those released by production and manufacturing processes, discharges from POTWs, and inadvertent releases from fossil fuel combustion. In a rural agricultural area the pollutant list is likely to include substances released from use activities e.g., pesticides, contaminants in fertilizers.

The ultimate goal of the exposure assessment is to develop site-specific control strategies based on the study's conclusions. Therefore, to streamline the process, the final list may contain certain pollutants that are representative of a group of substance. For example, a recommended control for an industry discharging a particular organic substance might be implementation of biological waste water treatment; this control would also be effective in removing other biodegradable pollutants present in the waste stream. The selection of one pollutant which adequately represents an entire group will require detailed preliminary knowledge of the local industries' waste characteristics and treatment efficiencies. However, this approach may overlook differences in exposure or toxicity between related substances.

The number of pollutants to select for study in a geographic exposure assessment will depend on budget, time and personnel constraints as well as on the particular focus of the study. In some cases, it may be appropriate to collect some categories of data on a large number of pollutants, particularly source emissions data which are derived from the same general sources for most pollutants. The number of pollutants which can be addressed in the environmental pathways analysis and exposure assessment, however, may be a subset of the initial list due to the substantial time and labor costs as well as the chemical-specific nature of the data retrieval and modelling required by these tasks.

Presented below is an outline of a step-by-step methodology for pollutant selection. The ordering of the steps may be reversed in some cases, e.g., input from local sources may enter at an earlier stage, serving more as a preliminary screening than as a reviewing function.

1) Compilation of a preliminary list of pollutants based on review of available government surveys of local industries and other sources, state documents on sources and emissions based on registration and permit data, other available Federal, region, state and local information published, unpublished, or based on personal communication.

2) For each pollutant on the preliminary list, compilation of general information of the following type:

- number of industrial and other direct sources;
- identification of other indirect sources based on nonlocal information (e.g., Intermedia Toxics List rationale, EPA Criterion Documents, EPA Effluent Guidelines Documents);
- quantification of emissions if data are available;
- readily available ambient air and/or water monitoring data for the geographic location (e.g., from STORET, state air quality surveys)
- designation on EPA special toxics lists, e.g., Intermedia Toxics List, Priority Pollutant List, Carcinogen Assessment Group's "hit list", Regional Toxic Substance Policy Committee Screening results, and other lists.
- anecdotal local information on spills, reports of problems and other episodes.

3) Review by EPA Region staff and any other interested local reviewers.

4) Selection of a list of pollutants to be addressed in the geographic study based on preceeding criteria; the number of pollutants selected will be based on the particular study's level of effort.

It should be emphasized again that the criteria implemented in the methodology for pollutant selection should not be rigid because of the inadequacies and inconsistencies typical of readily available data. The procedure should also allow the inclusion of qualitative information which may exist only for a few of the pollutants on the preliminary list, or which may be available only in selected geographic areas.

2.5 PROCEDURES FOR INITIAL SCAN

2.5.1 Initial Scan of Sources and Emissions

The initial scan of sources and emissions begins as soon as the information from the data acquisition effort becomes available. The objective of the scan is to determine the relative importance of the identified source/discharge modes and to identify other potentially significant source/discharge modes that may have been previously discounted. Some source/discharge modes previously assumed to be important will be dropped from further consideration if emissions are insignificant. The output from this effort will be a preliminary matrix of significant sources and discharge modes, compilation of estimated emissions for each source/discharge mode, and a rough map showing the location of the identified sources. This output will be used as input to the detailed source and emissions inventory (Chapter 3). In addition, the output of the initial scan of sources and emissions will be used as preliminary input to the study boundary definition, pollutant selection, environmental pathway analysis, and determination of exposure routes.

Before the initial scan takes place, the investigators should familiarize themselves with the toxics to be studied. Of particular importance with regard to sources and emissions is the acquisition of general information on the production, use, and environmental emissions of the toxics. With this information, a list of all possible sources of the toxic can be compiled, together with the possible discharge modes. All of the source/discharge modes included in this "master list" should be investigated with respect to the study area at some point in the initial scan or during the quantification of emissions, in order to ensure that no significant sources of toxics are neglected. In the event that the geographic approach to toxics control is undertaken on a large scale, it may be advisable for the EPA to assemble such a "master list" for each toxic of concern. This list and supporting information could be distributed to groups conducting geographic studies of toxics, thereby avoiding the duplication of time and effort.

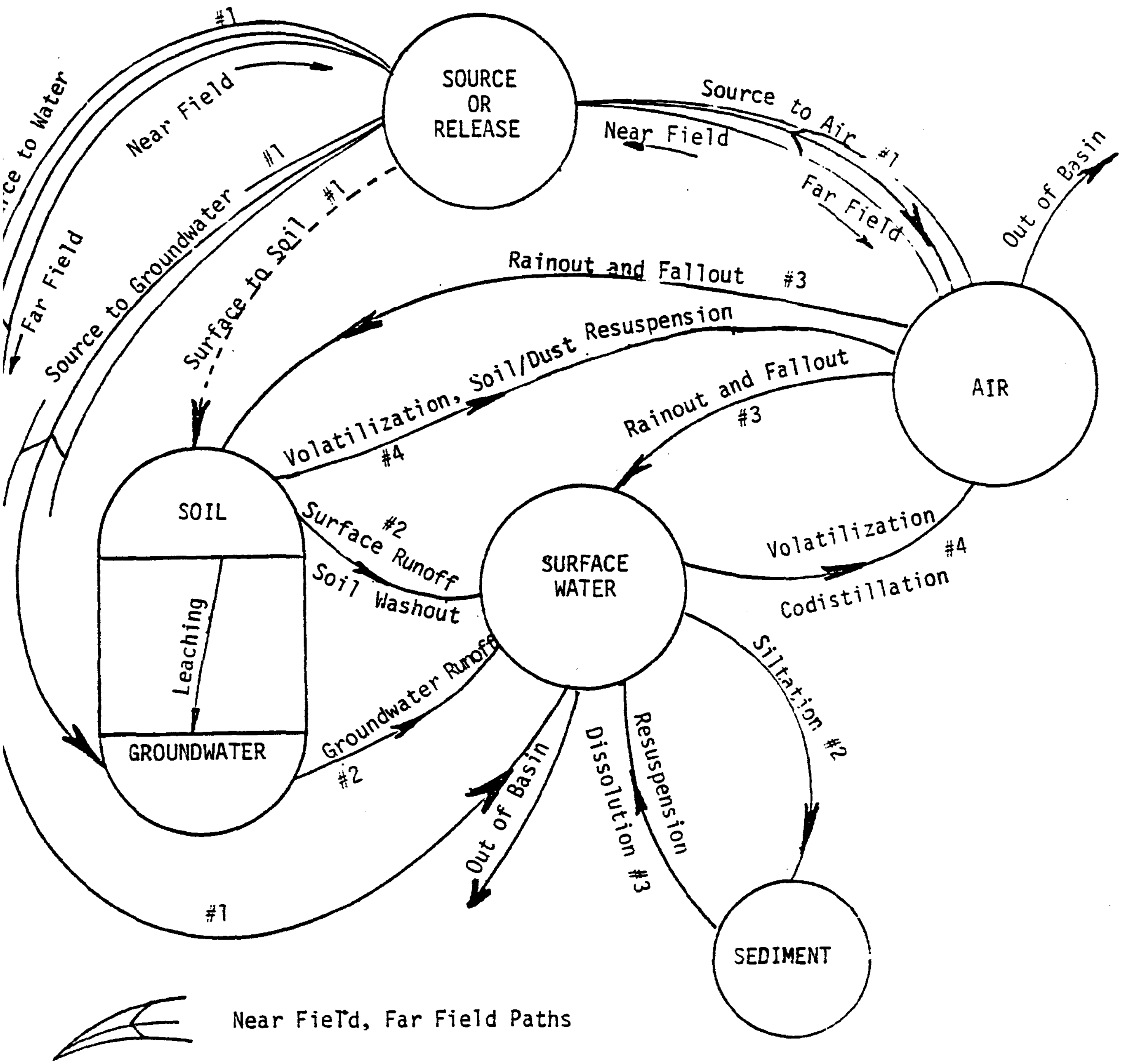
The following types of information should be sought in the initial data scan, as they will generally provide useful information on sources and emissions of toxics:

- Detailed land use information.
- Location of all potential sources of toxics (using the "master list" as a guide).
- A list of all industries in the study area.
- Qualitative information that can be used to confirm the presence or absence of toxics in identified potential toxics sources.
- Quantitative data that can be used to estimate emission rates from potential sources.
- Data on ambient levels of toxics in all media for sites outside the study that can be used to estimate imports of toxics to the study area.

Whenever possible, the data collected in the initial scan should be site-specific (i.e., pertaining to sources and emissions in the study area). When site-specific information is not available, however, regional data should be compiled; generic (i.e., regional or national) data are recommended if no other data are available. Some possible sources of data are described in Section 2.3 above.

2.5.2 Environmental Pathways Scan

Environmental pollution is mainly man-made and originates from point or non-point sources. Pollutants originating from these sources follow various environmental pathways and result in pollutant concentration levels in the three major physical environmental media: air, soil and water. Figure 2-2 is a schematic presentation of potential pathways of toxic substances originating from a source and discharged into any of the three receiving media (designated as compartments) of air, soil and water. In this figure, sediment is part of the water in the soil compartment, groundwater is part of the soil compartment, and biologic degradation can take place in any compartment. Each major environmental compartment may further export pollutants to a compartment of the same nature (i.e., out-of-basin transport), although such details are difficult to present in this type of schematic figure.



- #'s indicate priority of pathway
- #1: Direct Discharge Pathway
- #2-4: Indirect Discharge Pathway (primary, secondary, potential)
- Degradation of toxic substances can occur in any compartment

FIGURE 2.2: ENVIRONMENTAL PATHWAYS OF TOXIC SUBSTANCES

Pollutant pathways can be classified into two major categories:

(1) Direct discharge pathways created by the direct release of substances into the three major environmental compartments; for example, source-to-air pathway; and

(2) Intermedia transfer pathways created by the migration of substances between the three previously described compartments; for example, the air-to-surface pathway.

In addition, direct discharge pathways may consist of a near-field and a far-field subpathway (see Section 4.4). Potential pathways of toxic substances have been numbered from 1 through 11 in Figure 4-2. Individual and integrated modeling of these pathways is discussed in Chapter 4.

Compartments can be prioritized by examining the characteristics of the specific site. Intermedia transfer pathways can then be identified as having high, moderate, or low importance. The crucial compartments and pathways will depend on the nature of the sources (e.g., location, release mechanism and media), the pollutants present at a site (e.g., soluble, reactive), the exposed population (e.g., size, location), and the nature of the site (e.g., mountainous, coastal).

Table 2-2 outlines some specific considerations previously discussed. Examination of these factors for a site will lead to a conclusion as to which media must be modeled, and which pathways and media are likely to be of secondary importance. For instance, in the pilot study of the Kanawha Valley* the major discharges were from industrial sources by stacks (air) and river outfalls (water). Thus, air and water were important media, and important pathways were air-to-surface-to-water and water-to-air. Since the drinking water in this region came

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*see footnote, page 1-1.

Table 2-2

OUTLINE OF CONSIDERATIONS USED IN IDENTIFYING IMPORTANT PATHWAYS AND MEDIA

1. Nature of Emission Sources
   - Types of sources: point, non-point, area, line, volume
   - Mode of emissions: continuous constant rate intermittent batch operations, continuous operation but variable emission rate
   - Range in emission rates: significance of individual sources vs. source aggregation
   - Release mechanisms
   - Release medium

2. Nature of Emitted Substances
   - Toxic substance emitted directly
   - Toxic substance precursor emitted
   - Importance of physical, chemical, biological removal mechanisms
   - "Order" of chemical removal mechanisms: inert, first-order (simple exponential decay), or higher order

3. Nature of Exppsure Populations
   - Distribution
   - Near-field/far-field of sources
   - Long-term (chronic) exposure vs. short-term (acute) exposure
   - Statistical average or mean conditions vs. extreme "worst-case" conditions
   - Direct exposure to toxic in media vs. loss to other media and pathways
   - Routes of exposure, inhalation, ingestion, etc.

4. Nature of Site
   - Geography: mountains, coastal plain, valley, etc.
   - Special meteorological features: wind channeling in valleys, sea breezes, extremes of temperature, rainfall
   - Representativeness of available meteorological data
   - Significance of "imported" or "background" levels of toxic substance with respect to boundaries of study area and air basin
   - Soil types
   - Biota types and distribution

primarily from water resource supplies outside the study area, contamination of groundwater was of less concern. In another site, for example, in a community with drinking water wells near a hazardous waste disposal site, the soil and groundwater media and pathways might have been of primary importance.

Once the major pathways and media are identified, the required temporal and spatial distribution of the pathway analysis results can be specified. These considerations will depend on the nature of the sources (continuous, batch operation), the nature of the exposed population (area of affected population, use patterns of media), and the focus of the study (chronic versus acute effects). After the areas of study and the type of results needed have been determined, the use of actual models and analysis of existing data can be designed to satisfy the study objectives.

2.5.3 Exposure Route Scan

It is unlikely that it will be possible to identify and quantify every potential exposure pathway for toxics in a particular region within the scope of a study. Therefore, one of the first steps in a regional exposure assessment is to narrow the focus of the study to encompass only the critical exposure pathways for each pollutant. The final decisions will usually be based on limited, preliminary data for the area; however, in most cases these data will be adequate to support the initial screening.

Several types of data are useful in identifying exposures. The particular set of pollutants selected for the regional study will determine whether exposure through product use (e.g., of pesticides) is important and in what environmental media the pollutants are likely to concentrate following release (e.g., sediment for substances with propensity for adsorption). The types of pollutant sources present--industrial, commercial and domestic--will also influence the exposure pathways which are most significant in a region. For example, sources with ambient temperature releases from low stacks and vents are more likely to have an impact on the immediately surrounding population than are high temperature sources with tall stacks. Following specification of the study area boundaries, some of the immediately apparent regional characteristics, such as gross population distribution, the presence of recreational areas, or the type of water supply, will also aid in identification of critical exposure pathways. For example, in studying trace metal emissions, remotely-located smelters may be of less interest than coal-fired power plants sited in populous areas due to the lower exposed population associated with remote locations.

Concurrently with the selection of critical exposure routes, a decision should be made regarding which receptor categories to consider in the study area and at what level of detail they should be grouped. This choice is once again dependent on the variables discussed above. A quick survey of the types of receptors (populations by species), habitat or community, etc.) present in the area will indicate the presence of sensitive or endangered communities or habitats, economically or otherwise important receptors (crops, game species), large fractions of potentially sensitive receptors (elderly, children, pregnant women), as well as other information.

Once the critical exposure pathways and receptors have been identified, the next step in the assessment is to gather and evaluate more detailed quantitative information for these elements to use in estimating exposure levels. Chapter 5 discusses a general methodology for developing intake and population data.

2.6 OUTPUT OF INITIAL SCAN

The results of the initial scan will be an identification of the selected pollutants, sources, environmental media, and receptors to be considered in the subsequent analysis. These results can be conveniently displayed within the pentagram framework, as illustrated in Figure 2-2, extracted from the pilot study of the Kanawha Valley (see footnote, p.1-1). Four pollutants were selected in this study to be investigated in detail for possible linkages between source emissions and receptor exposures. These were lead, chloroform, carbon tetrachloride, and vinyl chloride. Emissions of these substances are indicated for four major source categories: industrial, POTW, coal mines, and POTW's. The dots in Figure 2-3 indicate that lead emissions were considered in all four categories, chloroform emissions were considered in both industrial and POTW sources, and the other two chemicals were identified only in industrial emissions.

The next segment of the pentagram, moving counterclockwise, indicates the receiving media that were considered for each source category. Industrial emissions were addressed for air, water, and land; POTW emissions for water only; coal mine emissions for water and land, and transportation emissions for air only. It is important to note that these restrictions reflect priorities that were established as a result of the initial scan; there were in fact other less significant routes of toxics entering the environment that were not addressed in the detailed Phase 2 analysis. This is true of the next segment also, in which environmental fate and transport mechanisms were considered. As indicated by the dots in Figure 2-2, attention was focused on transfers from air and land to surface water; from surface water to drinking water, biota, and air; and also deposition from air to land. Of course, the mass fraction of pollutant remaining in each receiving medium was a primary consideration.

The next segment of the pentagram indicates the exposure routes which were given highest priority for further investigation. Exposure of humans was considered with respect to all five environmental

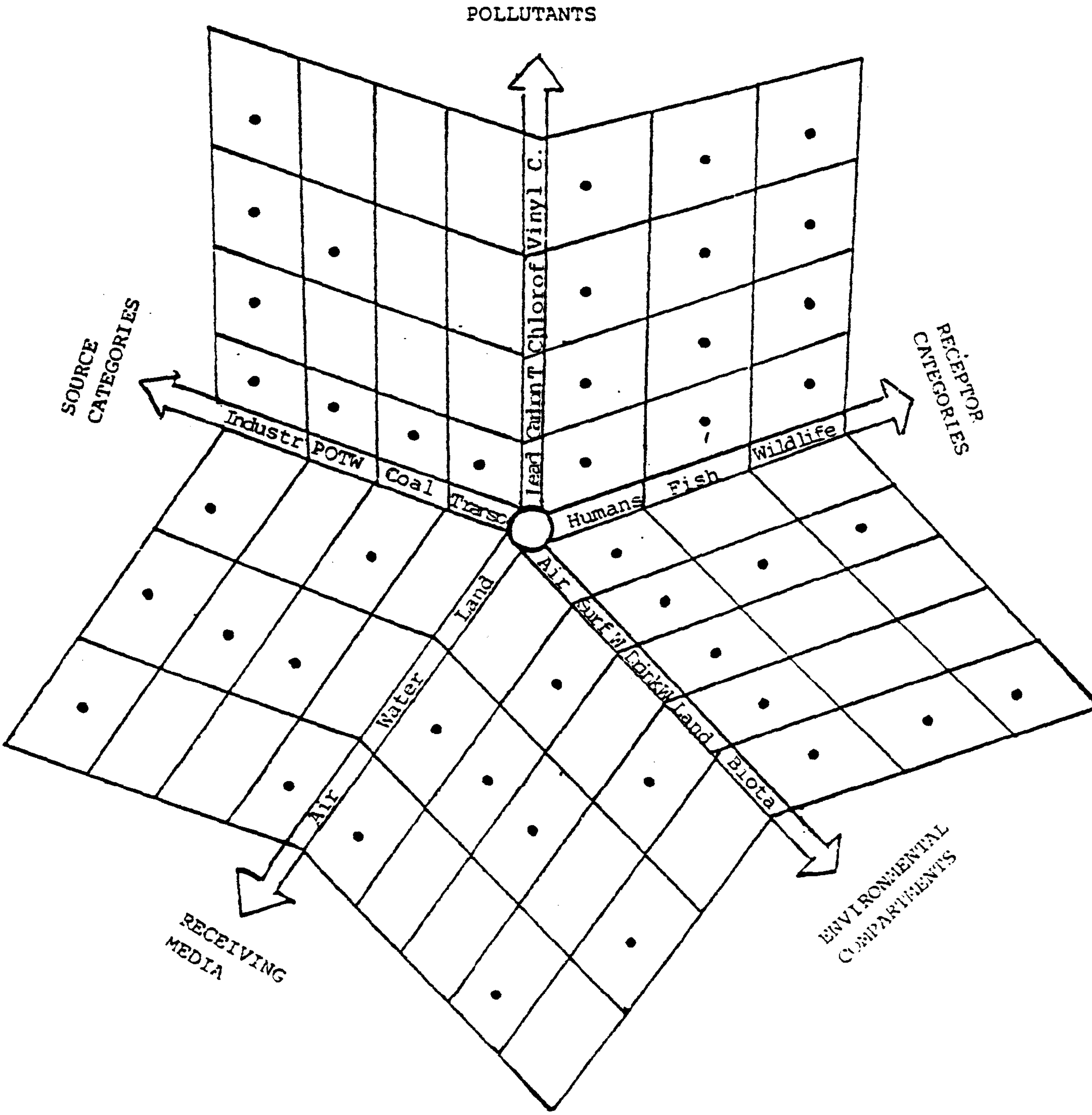


FIGURE 2-3: RESULTS OF KANAWHA VALLEY INITIAL SCAN

compartments--air, surface water, drinking water, land, and biota. For fish and wildlife, the only exposure routes considered were via surface water and other biota. Finally, the fifth segment shows that all three receptor categories may be exposed to any of the four pollutants, since a multiplicity of pathways exists from sources to receptors. Thus, each dotted cell in the pentagram defines a unit of technical analysis that will be pursued in the subsequent Phase 2 effort. This device serves both to display the output of the initial scan and to guide the conduct of the exposure analysis.

3.0 IDENTIFICATION OF SOURCES AND QUANTIFICATION OF EMISSIONS

3.1 INTRODUCTION

The cornerstone of an effective exposure assessment is a thorough identification of all significant sources of the toxics of concern and quantification of emission rates via each discharge mode. These components form the basis for all the succeeding phases of the exposure assessment. In addition, because most control strategies are oriented to control of the source, accurate characterization of emissions is vital to the overall success of the geographic approach.

The pentagram framework for exposure assessment, described in Chapter 1, provides a conceptual framework in which identification of sources and quantification of emissions occupy the first two grids in the pentagram. In practice, the two components are addressed concurrently; all sources with non-zero emission rates are potentially significant. Because of the close association of the source identification and emissions quantification, they are discussed together in the following pages.

The principal subtasks required to complete a sources and emissions inventory are:

1. Define data needs
2. Review and assemble existing data
3. Evaluate adequacy of existing data
4. Design and implement program for collecting new data
5. Synthesize and interpret data

Each of these elements are discussed in detail in the following subsections.

3.2 DEFINE DATA NEEDS

The initial subtask in the sources and emissions inventory is to define the minimum set of data that will be required to provide the needed levels of resolution and accuracy. As the foundation of all the succeeding tasks in the exposure assessment and the most likely point in the source-exposure chain for control strategy development, the source and emissions inventory must be as accurate as possible. Given the resource constraints that afflict all scientific studies, however, some balance must be struck between the optimal level of accuracy and the level that can be considered adequate to ensure valid results.

Because of the intrinsically site-specific nature of the geographic approach and anticipated variance in resources available to conduct geographic studies at different sites, it is not reasonable to set across-the-board standards for the minimum data set required. Nevertheless, the major considerations in defining data needs will be the same for all sites. These are:

1. Scope of exposure scenarios. The primary feature of the geographic approach is that it engenders site-specific analysis of exposure via ambient (e.g., air and water), and drinking water scenarios. The ambient scenario includes exposure related to waste disposal, transportation (spills), and several other components such as atmospheric or riverine imports. The three other scenarios considered by EPA's Exposure Evaluation Division (EED, Office of Pesticides and Toxic Substances), occupational, consumer, and food, can be integrated into the analysis but the marginal benefits of including these scenarios may be negligible. EPA's jurisdiction in controlling occupational and consumer exposure is limited. Locally grown foodstuffs, such as homegrown vegetables and fish, are probably worth considering as potentially important vehicles of exposure due to locally controllable toxics problems; food "imported" from outside of the study area may not be effectively addressed by a geographic study. Therefore, it is anticipated that sources of ambient exposure (industrial discharges, commercial emissions, etc.), drinking water exposure (ground water contamination, haloform reaction, etc.), transportation-related exposure (spills), and waste

disposal exposure (publicaly-owned treatment works, landfills, etc.) will be the primary focus of the emissions inventory. Food, occupational, and consumer scenarios may be partly or fully included depending on the nature of the toxics studied, resources available, and prospects for interagency coordination.

2. Age of data. Depending on how static or dynamic emissions rates are for given sources, some date must be set as the limit for accepting data as representative. This may be different for different sources. For instance, for an industry which installed new water treatment systems in 1979 due to BAT, the oldest acceptable data may be for 1980; for abandoned mine discharges, which might be suspected to have relatively constant discharges, the oldest acceptable data could be for 1974.

3. Site-specific data vs. regional or national data. Site-specific data are obviously preferred for geographic toxics studies but will often be unavailable or depauperate. In such cases, regional or national data on sources of toxics and average emissions rates could sometimes be used as a substitute, supplement, or quality control check. Substituting such data entails a risk of diluting the site-specificity of the approach but may be more cost-effective than sampling or making engineering estimates. The decision here must be based on the sensitivity of the overall exposure results to the emission rates in question; the relative costs of generating site-specific data as opposed to researching surrogate data; and the expected variability in emission rates with respect to time and location. It is anticipated that there will be large data gaps for many or most geographic study areas; because direct sampling may not be possible or cost-effective, it is recommended that EPA compile

some general catalogs of emissions rates for toxics that will commonly be studied. These catalogs could supply "fallback" values in the absence of site-specific data or be used as a basis for comparing site-specific emissions to emissions occurring elsewhere for quality control and general reference. Primary - information sources for regional or national emissions rates include exposure assessments and mass balances performed by EPA's EED (OPTS) and Monitoring and Data Support Division (Office of Water).

4. Variability in emissions rates. Many anthropogenic and natural phenomena controlling emissions rates are highly variable with respect to time and space. As examples, many industries discharge in "batches" due to discrete process steps; urban runoff occurs in conjunction with rainfall or snowmelt and the "first flush" usually carries the bulk of the pollutant load. To adequately characterize toxic loads, the distribution of emissions rates must be known with respect to any correlated variables (e.g., rainfall, number of batches per year, atmospheric inversions, flow, season, etc.). When defining the data set, the variability in emissions rates from different sources needs to be considered as a prime factor in determining the adequacy of data in representing the range of conditions which obtain at the site. "Worst case" and "average" scenarios can only be valid if these parametric relationships can be described.

5. Minimum number of samples required to represent emissions. The final consideration is the classic quality assurance problem: how many samples are needed to provide a reasonable representation of actual conditions? Unfortunately, the answer to this question is usually determined more by what the budget allows than by what the statistician desires. Primary factors in addressing this problem are related to the preceding considerations, i.e., are corroborating data or surrogate (fallback) data

available from regional or national studies?; what is the temporal and spatial variability in the emission rates?; are the data current?; etc. In some cases, mass balance calculations or other indirect means of estimating emissions can be considered as a substitute for direct sampling.

These five considerations for defining the required data set all entail a balance between the rigors of scientific defensibility and the constraints of manpower and funding limitations. A first cut at defining the required data set must be based on the judgment of the study team and the information collected in the initial scan. This target may need to be modified as work progresses if it becomes evident that the original definition does not strike the necessary balance. Further development of guidelines and policies for data adequacy would be helpful in assuring the quality of future geographic studies; it is recommended that these guidelines be developed prior to large-scale adoption of the geographic approach.

It is vital to include the personnel involved in the other exposure analysis tasks (i.e., environmental pathway analysis, receptor/exposure route analysis) as well as those involved in control strategies evaluation when defining the data needs. This helps avoid delays and misunderstandings later on.

3.3 REVIEW AND ASSEMBLE EXISTING DATA

The next subtask in the source and emission inventory is to review and assemble existing data. For each toxic on the list of pollutants to be studied, the discharges to all environmental media must be quantified to the extent possible. A logical framework to organize the emissions data is to consider all discharge modes (e.g., to air, water, and land) for each family of sources (e.g., industry, residential, commercial, imports, mining). In most cases, emissions data are organized by discharge mode for each source, rather than by pollutant. For example, an industry's water discharge permit might require monitoring of five toxics and data on all five would be available from the same reports. This organization of the data reflects the legislative mandate for data collection as well as EPA's own internal structure, which is generally media-specific.

Procedures for reviewing and collecting data on sources and emissions to air, water, and land are discussed in Sections 3.3.1 - 3.3.3. It should be noted that, although toxics emissions via spills are discussed only with respect to land, the same data base can be used to evaluate discharges to air and water.

3.3.1 Airborne Emissions

The primary goal in compiling a suitable data base for airborne emissions is to compile emission rates for all quantifiable sources within a defined study area. Because these data are used for exposure assessment in a geographic toxics study, it is also necessary to obtain additional specifications associated with the emissions, such as exit velocity, exit temperature, inner stack diameter, stack height, and area source specifications. Meteorological data, including representative wind speed, wind direction, atmospheric stability, ambient temperature, and mixing height, are also needed to perform the dispersion modeling required for the exposure assessment.

Emissions data can be obtained from emission inventories developed for source-specific data, assumptions based on per capita considerations and generic emission rates for source categories. In an area that has a large number of emission sources, prioritization of source categories will be necessary to make the inventory assessment manageable. Although it may not be possible to obtain data on each source (or in some cases each category of sources for heavily industrialized metropolitan areas), through careful consideration of the sources accounting for an acceptably large amount of the expected totals, meaningful results can be obtained in a cost-effective manner. In attempting to thoroughly review all potential data sources, a point of diminishing returns will be reached. Considering the degree of uncertainty in exposure assessment, the emphasis should be placed on assuring that the sources expected to be the major emissions within the study area are adequately characterized.

A general approach recommended for obtaining a suitable data base of airborne emissions is described below. For each category, source specific and generic approaches are identified, as applicable. The types of applicable data, and their limitations, are explained as follows:

> <u>Source specific data</u> - Under the authority of the Clean Air Act, states regulate the emission of airborne pollutants. Emission inventories are compiled that include major sources of criteria pollutants (SO_2, NO_2, total suspended particulates, hydrocarbons, CO, ozone and lead), and also emissions of hazardous pollutants (asbestos, beryllium, mercury and vinyl chloride) and specific hydrocarbon compounds that could be considered toxic. It is important to note that there can be a wide range in the confidence of these data since they can be obtained in a number of ways, including the use of stack sampling, mass balance considerations, emission formulas or simply best engineering judgments.
>
> <u>Generic data</u> - There may be a large number of relatively small sources which, when taken as a whole, can be a significant factor in a toxics study. In this case, in lieu of source specific data, estimates often can be made using per capita considerations such as emissions associated with degreasing, printing, dry cleaning, architectural coating, etc. In some cases, these estimates can be made based on employee totals within Standard Industrial Classification codes rather than general population data. Generic emissions are generally treated as area sources, and have a considerable amount of uncertainty. A drawback of generic data is that the maximum impacts from the relatively large sources within these categories are not individually reviewed. Generic pointsources are another possibility. For sources such as gas stations, a distribution of point sources can be made in an area based upon the number of employees in each area, per capita data, sales, etc. This approach allows for a better evaluation of impacts near the sources. Availability of data on airborne toxics emissions is generally very limited. Nevertheless, some procedures can be used to maximize the utility of existing data. These procedures are discussed separately, for various sources, below. The relative importance of each of the sources will, of course, vary from pollutant to pollutant.

Availability of data on airborne toxics emissions is generally very limited. Nevertheless, some procedures can be used to maximize the utility of existing data. These procedures are discussed separately, for various sources, below. The relative importance of each of the sources will, of course, vary from pollutant to pollutant.

Industrial

Industrial sources of airborne emission of toxic pollutants include those emitted from stacks/vents and from fugitive releases (i.e., emissions not released from a conduit). To obtain information concerning these emissions, the following should be performed:

- Review state emission inventories mentioned by the state air quality control agency. Obtain the following data on a pollutant specific basis for each registered source that is quantified:

  - latitude/longitude
  - exit velocity
  - exit temperature
  - inner stack diameter
  - stack height
  - adjacent building heights (building wake considerations)
  - continuous or batch releases
  - maximum and annual average emission rates
  - hours per year of operation

- Review air quality permits for major sources identified in the study area to obtain operation limitations and additional data on emissions, including limits on production rates; hours of operation, control efficiencies, fuel restrictions, etc.

- Contact the environmental affairs departments of major industrial sources and utilities to attempt to obtain necessary data. It is also advisable to contact major sources in the study area to confirm that data being used in the data base are consistent with current operations.

- Computerized data bases such as the National Emissions Data Systems (NEDS), the Hazardous and Trace Emissions System (HATREMS), the Storage and Retrieval of Aerometric Data (SAROAD) systems and numerous other data sources are theoretically useful in identifying major sources and areas of high atmospheric concentrations. At this time, however, there are two major problems in using these data bases for a toxics study. The data are mostly associated with criteria pollutants rather than a wide range of toxics. In addition, the data bases are generally incomplete. It is recommended that these data bases be reviewed, but only as a supplementary measure.

Residential/Commercial

Emissions of toxic pollutants from the residential and commercial sectors can be significant when taken as a whole, even though individual contributions may be small. Because these sources are not usually addressed in inventories, as the industrial sources often are, quantification will generally involve a rough approximation. In addition, in evaluating exposure, these sources are often treated as area sources, which further adds uncertainty to the analysis.

A reasonable approach to the quantification of these sources includes the following elements:

Residential

- evaluate fuel use for home heating (e.g., natural gas, oil, coal).
- estimate emissions of toxics based on available emission factors (e.g., Shih et al. 1980, U.S. EPA 1977b).
- uniformly distribute emissions over major residential areas within study area, or base distribution on residential density.

Commercial

- Identify the source categories that are expected to emit significant quantities of toxic pollutants of interest to the study. Possible categories include:

  - gasoline marketing
  - degreasing
  - drycleaning
  - architectural surface coating
  - graphic arts
  - asphalt sources

- Obtain the most recent population data and project current levels.

- For source categories emitting significant quantities of toxic pollutants of interest to the study, quantification of emissions can be approximated by per capita factors.
- Determine if production data for relatively large sources in the commercial categories can be quantified. If so, these emissions should be subtracted from the per capita derived totals, and modeled as discrete sources.
- Distribute area source emissions on the basis of the density of commercial establishments within the study area. A simplified approach would be to uniformly distribute them over the central business district.

Mining

If product dust contains pollutants of interest to the study, the emissions assessment must consider emissions from blasting, handling, transfer, and storage of the products of the mines in the study area. Most data on emission factors appear to be available for coal. There are a number of references available that contain emission factors from mining. Region VIII of the U.S. Environmental Protection Agency has summarized several reports on the subject (U.S. EPA 1979g). Mineral processing facilities are a potential source of toxic airborne emissions that should also be considered. Mining and mineral processing facilities are covered by reporting requirements similar to those pertaining to industry in general. Use the same procedure as that outlined under "Industrial" to obtain information on this source.

Transportation

Transportation sources include automobiles and trucks, railroads, ships and aircraft. In general, the major source of emissions from this sector are road vehicles. Although the other sources should be considered in geographic toxic studies, the primary emphasis would usually be on gasoline and diesel fueled road vehicles. Emissions of toxic pollutants from automobiles include lead, benzene, toluene, asbestos and a wide variety of organic compounds. The composition of the exhaust from gasoline and diesel fueled road vehicles should be considered in order to determine if these emissions are significant to the study. The following describes a general approach to characterizing these emissions:

- From the state highway administration for the state in which the study area is located, obtain the most recent annual vehicle miles traveled (AVMT) data representative of the study area. Factoring may be required on the basis of population to extrapolate to the study area in question. In lieu of this information, fuel marketing data from tax records or per capita fuel use estimates may be used in determining AVMT in the study area.
- Emission rates (e.g., grams/km) may be obtained from references, such as Black et al. (1977).
- Define the area over which the AVMT will be distributed, given particular attention to the areas of maximum vehicular traffic.
- If justified on the basis of traffic flow within and through the study area and resources allocated to the study, major routes may be treated separately for the emissions assessment and dispersion modeling analysis. Additional information such as road width, average speeds travelled, and maximum usage rates should be obtained if this approach is deemed necessary.

Imports of Toxics and Biogenic Production

In addition to the above sources, some toxics may be advected into the study area (imported) from other areas (e.g., PCBs) or may actually be produced biologically within the study area (e.g., phenol). Although it is anticipated that in most cases these sources will be negligible with respect to the others, these sources bear investigation. The best source of information would be actual monitoring data at points near the periphery of the study area (imports) or at the center and edges of populations suspected of synthesizing or metabolizing toxics. Clearly, such data are rarely available and can usually be regarded as low priority data gaps.

3.3.2 Aqueous Discharges

Aqueous discharges can be divided into non-point source and point source discharges. These are studied in fundamentally different ways, and so are discussed separately in the following pages.

Non-Point Source Water Discharges

The methodology for assessing the Non-Point Source (NPS) water discharge inputs of toxic substances to a geographical study area is dependent on the resources available for the project. Unlike point source discharges which are discretely identifiable and often do not vary considerably with time, NPS discharges are diffuse and subject to great variations dependent upon the meteorological conditions. In its simplest form, the methodology for assessing NPS water inputs to the geographical study area is dependent on site specific data for rainfall, runoff (hydrology), land use, and water quality concentrations that are averaged over some time period, such as a season or an entire year. In its complex form, the NPS input methodology must account for the ambient meteorological factors that affect runoff, water quality, and resulting pollutant loads. These factors include rainfall intensity, duration, wind velocity, solar radiation, antecedent moisture conditions, and time of year. In addition, land use characteristics such as basin and channel slopes, soil types, impervious areas, stream channel characteristics and the basin's anthropogenic activities must be considered. The complex methodology would generally require the use of a sophisticated computer modeling package (e.g., U.S. EPA SWMM model), which would require pre-calibration with site specific data before the model could be run to generate predicted pollutant loads. Considering the limited data base currently available on toxic substances in NPS water discharges, this approach is probably unwarranted unless the resources are made available to fill the existing data gaps. Therefore, the methodology addressed in the following discussion is much more practical and simple in scope, and designed to provide general estimates of the possible magnitudes of NPS toxic loads. The methodology consists of five steps.

- <u>Define Study Area by Subwatersheds</u>

  The first step required in the NPS assessment effort is the definition of the study area according to surface water drainage patterns. Consider only those basins that drain directly into the study area. Ideally, basins identified should be small enough that sources of pollutants may be readily identified according to some land use activity or pattern.

This is particularly important in areas where the land use is particularly diverse. Not only will the use of small drainage basins permit the identification of pollutant sources, it will also define the study area according to a source control pattern if control measures are required. In some cases where geographical study areas occupy the mid section of large river basins, it will be necessary to consider the NPS inputs of major tributaries and upstream reaches under the source category of imports. This method involves the use of river discharge records and in-stream water quality to estimate toxic pollutant import loads, and is discussed in greater detail with point source water discharges.

- <u>Collect Land Use Data</u>

  Once the study area has been defined according to surface water drainage basins, the collection of the specific land use data is required. Generally, NPS discharges are grouped according to the following land use categories:

  - Agriculture
  - Silviculture
  - Urban
  - Construction
  - Mining

  Each of these categories could be further subdivided (e.g., urban-residential, industrial, commercial); however, detailed land use information is usually limited. Moreover, considering that water quality data are usually also limited, the allocation of considerable manpower and resources towards a detailed land use characterization is usually unwarranted. Total acreage for each of the land use categories chosen should be obtained for each of the identified drainage basins included in the study area.

- <u>Determine Runoff Yield</u>

  The next step is to acquire data on runoff. Ideally, a previous study effort may have already conducted instream sampling and water quality monitoring according to land use characteristics in the study area (such as studies conducted under Section 208 of the Water Pollution Control Act). Efforts of this type will frequently generate surface runoff yields for some time frame (e.g., gallons/acre/year) according to the major land use categories. Total basin seasonal or yearly flows are calculated by multiplying the area yield flow rate for each land use category by the area in each land use and summing accordingly. Alternatively, total flows for each land use category may be allowed to stand alone to permit toxic load calculation according to land use rather than according to individual subwatersheds. In the absence of area yield flows, use predictive runoff formulas that incorporate data on rainfall volumes and land use characteristics. The "rational" formula, for example, is commonly used for average runoff predictions, particularly in urban areas. The rational formula is:

$$Q = CiA$$

where Q = flow, C is a unitless runoff coefficient, i is rainfall intensity over time of concentration, and A is the area of the watershed. Values for the variables i and A are available from many sources, including the U.S. Geological Survey and the National Weather Service, and can be easily estimated from rainfall records and topographic maps. The runoff coefficient, C, varies as a function of the permeability of the watershed surface. Values for C are listed in standard hydraulic engineering texts such as "The Manual on the Design and Construction of Sanitary and Storm Sewers" (ASCE 1960). The accuracy of prediction can be increased by the use of the Soil Conservation Service (SCS) formulas, particularly for agricultural or other non-urban watersheds. Detailed information on runoff prediction using the SCS formulas is available in the "National Engineering Handbook-Hydrology" (Mokus 1972).

- Obtain Concentration Data

Obtain data on the levels of toxics in runoff so that pollutant loads can be calculated. This step is usually the most difficult. Site-specific water quality data are preferred; however, non-point source toxic monitoring has been extremely limited. It may be possible to locate heavy metal concentrations and pesticide data from previous "208" water quality programs in the geographic area. Toxic organic monitoring data are virtually nonexistent, and only crude estimates of pollutant loads are presently possible. In the absence of site specific data for aqueous concentrations of toxic substances, generic data may be substituted in order to calculate pollutant load estimates. The estimates generated for generic data should be clearly identified as such, however, and it should be understood that they may not represent conditions in the study area. Regardless of the data source it is important that average stormwater quality concentrations, rather than discrete or grab sample data, be used. Use concentrations that have been recorded as a result of flow-weighted sampling if available. This is because toxics concentrations may vary by several orders of magnitude across a storm hydrograph (particularly in urban areas that exhibit a "first flush" phenomenon) and discrete concentrations may significantly over- or underestimate a pollutants' presence.

- Calculate Pollutant Loads

  The basic method used to calculate loadings is simply to multiply concentration of a given pollutant times the flow. Pollutant load rate is thus expressed in units of mass per unit of time. Ideally, NPS loads are estimated for runoff from a series of typical storms occurring over the geographical study area during some time period such as a season or a year. Water quality concentrations that are seasonally recorded are therefore used. This process, however, may be extremely time consuming and considering the generally limited data base, it may be best to calculate total average yearly flow for each basin in the study area and multiply this by the average pollutant concentration to obtain a yearly loading rate for each land use category, as well as for each subwatershed. Total annual pollutant load in the study area is the sum of the individual subwatershed loads.

One alternative method of calculating NPS pollutant loads that eliminates the need for water quality and average flow data is the use of area yield pollutant loading rates according to land use. These data are extremely limited and will only have been generated as a result of a previous site-specific non-point source monitoring effort (such as a "208" study). Area yield loading rates express individual pollutant loads according to some measure of area and according to land use. For example, the area yield loading rate of lead for a particular urban area may be expressed as kilograms per hectare of surface area per year (kg/ha/yr). Similar yield loading rates may also be available from agricultural, silvicultural and mining areas. If accurate land use data are available, calculate the pollutant load by simply multiplying the area of a particular land use by the area-yield rate. Pollutant loads may, therefore, be expressed according to land use, or the individual land use loads may be summed to find the total watershed load, which in turn may be summed to calculate the total load for the geographical study area. Data of this type are not usually available, however.

Several other methods of estimating NPS pollutant loads are also available and may be used for making qualitative assessments. For example, if data on pollutant concentrations in runoff are not available, but flows and concentrations have been measured at ambient stations upstream and downstream of a study area, the following approach may be used: during dry periods, the difference between the pollutant load in the upstream station and the pollutant load in the downstream station can be assumed to result from loading from point sources; this loading rate can be assumed to be relatively constant. The upstream and downstream loads are then compared during storm events. The difference in upstream and downstream loads, minus the "baseline" point source load, can be considered to represent the load from non-point sources. This method of calculating the NPS pollutant load would have to be performed over several storm events of differing magnitudes in order to determine an average load.

Although the methodologies discussed above are relatively crude, the NPS data base for most of the priority pollutants is not sufficient to warrant a more sophisticated approach. Frequently, only a qualitative assessment is possible, based on land use activities, fate processes affecting the residence and transport of pollutants in the aquatic environment, and meteorologic processes that may affect NPS loadings. The state-of-the-art with regard to NPS studies and methodologies is currently in a period of transition. As a result of ongoing sampling programs and previous monitoring efforts (e.g., Section 208 studies), NPS pollution is being given more consideration as a significant discharge mode. As the NPS data base increases in size and the state-of-the-art advances, it is expected that improved methods will be developed for assessing the magnitude of NPS pollutant loads in a given geographical area.

Point Source Water Discharges

The existing data base for assessing point source water discharges of toxics in a geographic study area may often be more complete and quantitative than the data bases for other discharge modes. This is largely a result of the U.S. EPA National Pollution Discharge Elimination System (NPDES) and effluent guidelines sampling efforts. In the near future, data retrieval for NPDES will become even more streamlined with the advent of a new computerized system for NPDES records. It must be emphasized, however, that the toxics on the list of 129 "priority pollutants" have been given considerably more attention in previous sampling and monitoring programs than have other toxics; it is likely that a geographic study of non-priority toxics would require significant amounts of new data. A detailed discussion of the recommended methodology for assessing point source toxic discharges is given below, followed by methods for evaluating imports of toxics via waterways.

After completing the initial scan, the location of most sources of toxics data will already be known and preliminary data gathering efforts will have been completed. For point source water discharges, the bulk of the pertinent site-specific data will be located at the regional EPA office (with personnel responsible for enforcement), at the state office responsible for water discharge permits, with the permit-holders or, in some cases, with the U.S. EPA National Enforcement Investigation Center (NEIC). The Effluent Guidelines Division of EPA headquarters will be the most knowledgeable source for non-site-specific (i.e., generic) data.

As one of the first steps in assembling existing data, obtain a list of all NPDES and state water discharge permit holders should be obtained for the geographic study area. There are several computerized data bases that will provide the NPDES list. Currently the U.S. EPA IFD (Industrial Facility Discharge) file is the most suitable, as it will provide a list of NPDES permit holders for a whole USGS basin. If the study area does not correspond to a basin, make a computer retrieval for all basins in which the study area is located. In this case, permit holders outside the study area can be eliminated from the list on the basis of location (latitude/longitude). In addition to location, the IFD retrieval provides useful information on the NPDES permit number, effluent flow, Standard Industrial Classification (SIC) code, and receiving stream. In the near future a new computerized NPDES file will be available, which may be more useful than the IFD file; this system will provide data on pollutants requiring periodic monitoring in addition to most of the information available in the IFD file. The list of state water discharge permit holders in the study area may be obtained either from responsible state personnel or by going through the state permit files. Depending on the size of the study area and the organization of the files, however, the latter option may be very time-consuming.

Once the list of all state and NPDES permit holders is assembled it should be divided into several subcategories based on the likelihood that individual sources contribute the toxics of interest in the study. Based on discussions with knowledgeable federal and state personnel, a high priority list should be compiled. Initially, the permit holders in this category should include all "major" dischargers (as determined by a ranking system used by U.S. EPA), all 34 "primary" consent decree industries, and all other dischargers suspected of discharging the toxics. By examining available records, this list can then be pared down to those facilities known to discharge the toxic, based on discharge monitoring reports (DMRs) or other sampling results. The permit holders culled from this high priority list that are suspected of being sources of the toxics of interest can be placed in the second category along with other permit holders that are suspected for any reason to be potential sources of the toxics. All permit holders that are not potential sources of the toxic can be placed in the third, low priority, category. As a general rule, only the first two categories need be investigated further.

In order to assess the contribution of toxics from each of the known or suspected sources, information on effluent flow, toxics concentration, type of discharge, and operating schedule must be obtained. Because the sources of information and calculations are different for the "known" and "suspected" dischargers, these categories will be discussed separately. Effluent flows for the known contributors of toxics will generally be available from one or more of the following sources: state and NPDES discharge monitoring reports (DMRs), IFD file, NPDES or state discharge permit applications, reports of NEIC investigations. Usually the range of flows and the mean daily flow will be available on a monthly basis for each outfall. The monthly records are preferable to all other data because they are generally more up-to-date. The toxics concentrations may be available from the DMRs, sampling results submitted to EPA and/or the state by the dischargers to fulfill permitting requirements, or sampling conducted by the agencies themselves. If available, the DMRs are the best source of concentration data because they provide both a long-term flow-weighted average and a range of concentrations. Information on the type of discharge (e.g., batch, continuous), and the operating schedule (e.g., 16 hour-day, 350 days/yr) can usually be obtained from permit applications; otherwise, EPA and state personnel or reports may be helpful. Once the flow, concentrations, and flow characteristics are known, the toxics loadings can be estimated on a mass/time basis by multiplying the concentration by the flow times the appropriate conversion factors. Both the average loadings and the range of loadings (e.g., "worst" case, "best" case) should be reported, if possible. The exact units will depend on the type of modelling planned for the exposure assessment. Existing source-specific data can be confirmed and new information obtained for the dischargers in the "known" category by contacting personnel and/or conducting effluent sampling, as discussed below for the "suspected" category.

Facilities in the "suspected" category, as mentioned previously, will include those for which no site-specific toxics data are available that belong to one of the 34 "primary" industry categories or are otherwise suspected of being dischargers of the toxics. Because this category, by definition, includes facilities for which there are considerable data gaps, these gaps must be filled in order to assess toxic loadings in plant effluents. The best way to fill the data gaps is to contact plant personnel. This should be done in an organized fashion beginning with a letter and followed up, if necessary, with a phone call. For many of these facilities the flow will be available through DMRs or permit applications. The facility should be requested to confirm flow estimates, as well as to voluntarily provide data on effluent toxics concentrations collected in self-monitoring (if available), and information on raw materials, products, and treatments-in-place. Obviously, the information requested should be tailored according to the data needed and the type of facility. Alternatively surrogate (national or regional) data can often be used to estimate primary pollutant toxics concentrations and, if necessary, flow characteristics. The Effluent Guidelines Division (EGD) of U.S. EPA is the best source of surrogate information for the 34 "primary" industries, because it has conducted effluent sampling of representative facilities for these industrial categories. This information is usually available in summarized form, by industry, in the "development documents" available through EGD. In addition, EGD has conducted selective effluent sampling of some industrial categories other than the 34 primary categories. Toxics loadings can be estimated for the sources in the suspected category in the same manner as for the known category. Loadings estimates, however, should be clearly designated as to whether they are based on site-specific data or surrogate data.

If the study area does not encompass the entire headwater portion of a hydrologic basin, estimates must be made of toxics imports into the study area via surface waters. Because these imports are conveyed in stream channels, they are discussed here as point sources. Consider each aquatic segment upstream of the study area as a potential point source of toxics entering the study area at the point where the study area boundary intersects the stream/river. In order to evaluate the toxic loadings from imports, collect ambient data on flows and toxics concentrations for all tributaries to the study area. These data may be available through the computerized EPA STORET file, or may be obtained directly from agencies that conducted the sampling (e.g., EPA, USGS, state agencies, U.S. Army Corps of Engineers). Once assembled, the data for each upstream segment can be compiled in the following manner. Calculate a separate loading (mass/time) for each sample taken, by multiplying the flow by the ambient toxic concentration. Calculate average loading and the range of loads from the individual data points. If the individual data points are not available, multiply the average flow by the average toxic concentration; however, this estimate will be less accurate than estimates using individual data points.

3.3.3 Discharges to Land

Discharges to land include landfilling, disposal in hazardous waste sites, sludge spreading, intentional application, and other activities. Existing information on toxics discharges to land will usually rely on RCRA manifests, treatment, storage, and disposal (TSD) permit applications, and related material. Although the advent of RCRA hazardous waste regulations has greatly increased the availability of data on land-destined disposal, this media is still one of the least-quantified for toxics. The sources of existing data can be discussed most logically with respect to the environmental pathways they cover, i.e., waste disposal, residual levels, or spills. Each of these are considered separately below.

Waste Disposal

Waste disposal on land can be separated into two sources of toxics: disposal of known hazardous waste and disposal of residential/commercial/ /industrial waste that may contain unknown amounts of toxics. For both of these waste categories two types of data are required to categorize the sources and emissions. First, the type of waste, its origin, quantity, and form should be known. Second, the location and method of disposal should be known. For known hazardous wastes the above data will often be available through state and federal hazardous waste control laws, regulations, and permits. For wastes with unknown amounts of toxics the data are more difficult to acquire. While information on quantitites of waste, generic waste types, and disposal of wastes is often readily available, data on the specific quantities of toxics in "ordinary" residential/ commercial/industrial wastes are usually unavailable.

Contact regional EPA hazardous waste sections, State hazardous waste disposal agencies, State health agencies, and local planning boards as the primary information sources. The types of information available from each of these organizations is listed in Table 3-1. This information should provide qualitative data on the general composition of wastes or the types of waste streams, and quantitative data on the total mass of wastes

Table 3-1

SOURCES OF DATA ON LAND-DESTINED DISPOSAL OF TOXICS

Source	Data Available
• U.S. EPA Regional Office	- RCRA Part A hazardous waste treatment, storage, or disposal permit application forms - RCRA Part A hazardous waste transportation manifests - RCRA Part B hazardous waste disposal site inspection forms - Investigative reports dealing with a hazardous waste disposal site or a source of hazardous waste - computerized data base with all RCRA application data
• State agency with responsibility for hazardous waste regulation	- hazardous waste disposal permits - hazardous waste site inspection forms, monitoring records - transportation manifests - knowledgeable personnel familiar with the study area - state investigative reports on hazardous wastes in the study area
• State and local agencies with responsibility for public health	- may have data on risk to public from disposal of hazardous wastes
• Regional planning agency	- waste disposal plan, may be part of comprehensive plan

generated at and hauled to different sites. Because the exact composition (by percent weight, volume, etc.) of most wastes is not known nor is it required under most existing hazardous waste regulations, high resolution of the amounts of specific compounds in waste streams will usually prove difficult or impossible. Stated differently, hazardous wastes are generally defined as such due to the presence of a hazardous material; regardless of whether the presence is in trace amounts or as a homogeneous phase, it is reported the same way. In most cases, then, the available data will only provide a range of possible values for the "flow" of hazardous wastes.

If the toxics of concern may be present in waste streams that are not designated as "hazardous," collect data on residential, commercial, or industrial wastes. Volume, composition, and destination of the wastes is required to characterize mass flow to the land compartment. Data sources for these "non-hazardous" wastes are listed in Table 3-2.

In all cases, collect any available information on waste containers, how long the sources have discharged the wastes, historical volumes of discharges, and other pertinent information.

Regional or national data may be an acceptable surrogate for site-specific data, depending on the target data needs defined in the previous subtask. Mass balances, engineering estimates, or actual sampling data should all be considered if actual site-specific data are lacking.

Residual

Residual toxics are those toxic pollutants that are found within the soil as a result of past toxic discharges or geologic processes. Sources of such residual toxics include pollutants in active or abandoned waste disposal sites; toxics that have settled or precipitated out of the air; and toxics that have been deposited by surface water and ground water. Data on such residuals are often unavailable. Where information on residuals exist, it is usually generic (i.e., not site-specific) in nature. Some potential data sources are described in Table 3-3.

Table 3-2

General Waste Disposal Data Sources

Source	Data Format
• State agency with responsibility for solid waste regulation	- disposal site permit and inspection forms - documents with information on the amount of toxics in solid waste - personnel with knowledge of study area
• Regional planning agency	- solid waste disposal plan, may be part of regional comprehensive plan - existing land use data
• Local/Municipal planning agency	- solid waste disposal plan, may be part of comprehensive plan - existing land use data
• U.S. EPA Headquarters and/or Regional Office	- reports on toxics in residential/commercial/industrial wastes.

Table 3-3

Residual Data Sources

Source	Data Available
• Waste disposal data sources (See *Waste Disposal*)	- data on abandoned and active disposal sites - information on past disposal practices
• Soil Conservation Service	- soil reports and analysis
• U.S. EPA Headquarters or Regional Office	- reports on ground water contamination and analysis of toxics in sediments.
• State agency responsible for ground water	- reports on ground water contamination.
• U.S. Army Corps of Engineers, State conservation or natural resource agency.	- analysis of toxics in sediments.

Data on residual toxics, especially organics, are generally even more limited than data on active waste disposal processes. Nevertheless, residuals can be quite significant, especially for refractory compounds such as PCBs or DDT, and act as a reservoir with potential for future releases. For ephemeral toxics, residuals are not important and can be disregarded.

Spills

Spills of hazardous wastes or toxics on land are often difficult to quantify because of a lack of data for past events, and inadequacies in the available data base. There are obvious reasons why many spills are never recorded, or at least never made public. Reports on spills are often sketchy as to details and may lack information on such activities as cleanup and disposal of the spilled toxics. Some potential sources of data are listed in Table 3-4.

Spills are intrinsically episodic and difficult to predict, so there is little potential for using national or regional data for all but the most frequent occurrences (e.g., loss during filling of oil tank trucks). Relating the source and emissions inventory to later exposure assessment tasks, most environmental models cannot realistically model spill events, and the utility of spills data in making quantitative predictions of exposure is not presently clear. Nevertheless, these occurrences can be extremely significant vehicles for exposure, especially for high volume industrial chemicals.

Table 3-4

Spill Data Sources

Sources	Data Format
• EPA Regional Office	Log of hazardous waste spills
• State agency with responsibility for hazardous wastes	Log of hazardous waste spills, data may be in separate company files
• State public health agency	Record of toxic substance spills

3.4 EVALUATE ADEQUACY OF EXISTING DATA

As work progresses with subtask 2, (assembly of existing data) compare the collected data with the data needs defined in subtask 1. It is important to periodically evaluate the adequacy of the existing data; do not wait until the end of the data collection phase because most of the measures employed to generate new data require considerable lead time. This evaluation represents a checkpoint on data quality and quantity--are there enough data, and were the original procedures used to produce the data sufficient to build upon for the exposure assessment and control strategy development?

The gaps between the desired quantity and quality of data and the available quantity and quality of data will often be large, particularly for airborne and land-destined emissions. Several measures are available to bridge these gaps (these are discussed in the next subsection), but most are costly relative to the effort involved in collecting and assembling existing data. Thus, when existing data are inadequate, the program manager is faced with a difficult decision: to proceed with the analysis and strongly caveat the results; to pour resources into further data collection; or to abandon analysis of certain pollutants or sources.

Two tools are available to assist in this decision: sensitivity analysis, and the environmental pathways models developed for the next phase of the exposure analysis (discussed more fully in Section 4 and Appendix A). Sensitivity analysis can be used to indicate how sensitive the total emissions "budget" is to inputs from a given source or group of sources. Inherent to this approach is the assumption that enough is known about the source to assign some range of toxics loadings that will bracket the actual loadings. The high end of the loading estimate is the critical one, and should be environmentally conservative (i.e., do not underestimate). Compare the estimated maximum load to the loads from other known sources. If the total load is sensitive to the estimated maximum load from the unknown or poorly quantified sources, further study is required. If total load is not sensitive, but temporal or spatial considerations indicate that the source may be an occasional acute problem or severe local problem, further study may also be required. If neither of these conditions obtain, it is unnecessary to acquire more data on the source(s).

A second and technically preferable tool is to use the models developed for the environmental pathways analysis. Provided that adequate ambient data are available, and that emissions are fairly well-defined for some sources, the available source data can be input, and resulting model predictions can be compared to measured ambient levels. If the input emission rates account for the observed ambient concentrations, it is reasonable to assume that other sources are negligible. If predicted concentrations are significantly lower than the actual ones, other sources may be significant. Comparison of monitoring and modeling data is given more complete treatment in Section 4.4, as a number of other inferences can be made using this procedure. It is a valuable tool for evaluating the adequacy of existing data, but has drawbacks in that complete ambient monitoring data must be available; at least some emission rates must be known, the modeling parameters must be previously calibrated and verified to the extent possible; and it is expensive.

Both of the tools discussed above can be used to screen out sources that are insignificant with reference to others. It is axiomatic that a screening procedure based on comparison of relative values must have some known values as a basis for comparison. In many cases, data for a given pollutant will be inadequate or unavailable for all sources, and thus neither of the above tools are useful. If this is the case, the data base must be expanded.

There is one other situation in which further data collection is unnecessary. This would occur if the emissions from a source do not enter any environmental pathway that could result in exposure to humans or other receptors. An example of this rare case would be where all of an industry's emissions go to a secured waste disposal site with no potential for volatilization, leaching, or otherwise re-entering the biosphere.

To summarize, further data collection is not necessary if:

- the target criteria for data needs are satisfied by the existing data, and
- ambient concentrations are accounted for by emissions from known sources, or
- it is very likely that sources for which the data are inadequate are negligible with respect to sources for which data are adequate or
- although emissions are not quantified, it is known that there is no potential for exposure to human or other receptors due to the characteristics of the discharge mode.

More data collection is necessary if:

- the target criteria for data needs are not satisfied by the existing data, and
- estimated maximum emissions from sources with inadequate data are potentially significant in terms of total emissions or occasional or localized exposure-related problems, or
- ambient concentrations are not accounted for by emissions from known sources, or
- inadequate data are available for all sources of a toxic.

3.5 DESIGN AND IMPLEMENT PROGRAM FOR COLLECTING NEW DATA

It is anticipated that in most geographic studies, existing data will not be adequate to characterize emissions for at least some sources (and often all sources). Designing and implementing a program for collecting new data will thus become an important part of the technical approach. Some measures to correct data deficiencies include:

1. more exhaustive search for existing data
2. sample and analyze emissions or ambient media samples
3. develop engineering estimates or mass balance calculations
4. use available surrogate data (national or regional)
5. adapt analogs, using similar compounds with known emission rates.

Each of these are described briefly below:

Exhaustive Data Search

Usually, the great majority of existing data will be available from the government agencies and industrial contacts discussed in Section 3.3. In some cases, however, universities, consulting firms, and others may have conducted studies that are not known or available to the aforementioned groups. Exhaustive searches of these potential sources may yield some information. It is anticipated that the marginal benefits of an exhaustive search will rarely outweigh the marginal costs with respect to a thorough search of the previously identified data bases.

Sample and Analyze Emissions or Ambient Media

This is the most direct, technically satisfying, and expensive alternative. It entails extensive planning, coordination, and analytical time, but, with proper design, provides the most useful data. Coordinate sampling efforts with other elements of the exposure assessment; simultaneous analysis of emissions and ambient levels at critical points helps establish a firm linkage in the source-exposure chain. The ambient sampling program should be coordinated with any ambient sampling that is needed for the evaluation of monitoring data (Section 4.4). Use surrogate data, mass balances, analogs, or other estimating techniques to help determine where to sample. Like any other sampling program, it is essential that quality control and quality assurance elements be incorporated into the procedures.

In addition to the typical air and water sampling schemes, consider sampling media that act as information integrators. For instance, when studying hydrophobic refractory compounds in aqueous discharges, sample sediment in depositing zones; if spills are suspected from a facility but normal discharges are reported to be of good quality, sample benthic invertebrates downstream of the plant (since most of the organisms in the community have a life-span of over a year, normal composition indicates lack of chronic or episodic pollution).

Sampling sediment and other environmental 'sinks' is an excellent indication of the presence and relative amounts of a toxic. If insignificant amounts of a toxic are found in a 'sink' for the particular compound, it may be safe to assume that the emission rates are insignificant (depending on locations of sampling sites, sources, environmental fates, persistence, etc.).

There are numerous references available on sample program design. None of these, however, deal with the range of possibilities that are encompassed by the geographic approach - all environmental media; scores of point, non-point, and mobile sources; temporal variations; interagency coordination; etc. This subject was only superficially addressed by the current study and requires considerable development as a major component of the geographic approach.

Develop Engineering Estimates or Mass Balances

For some industrial, commercial, and natural processes, it is possible to develop estimates of toxics emissions using known flows in process streams and known or assumed partitioning into various waste streams, products, or media. Although these calculations are helpful in generating order-of-magnitude estimates, they cannot usually account for temporal variability, which can be extremely important in terms of exposure. The basic elements of mass balances and engineering estimates are to identify all pertinent processes; describe the releases and products from each process; and estimate flows and concentrations of toxics emanating from each process.

These tools are useful for providing rough estimates of emissions of toxics, but because the accuracy of the estimates is usually low, they are best used to provide inputs to the sensitivity analysis described in the preceding subsection, or to augment monitoring data.

Use Available Surrogate Data

As previously mentioned, regional or national data on sources and emission rates can be used as a substitute or quality control check for inadequate site-specific data. Apply caution when using such data; toxics emissions are obviously quite variable from area to area. Data from the same geographical area are usually preferable to data from more distant regions.

Because it is anticipated that surrogate data will be valuable as "fallback" values, it is recommended that a general catalog of emission rates be generated for seldom-studied sources such as urban runoff, mine drainage, residential waste disposal, etc. This recommendation, first mentioned in section 3.2, would allow either initial input of the cataloged values (i.e., surrogate data would be initially defined as adequate to meet data needs) or after the data gathering phase, if inadequate site-specific data were available, it could be used as a "fallback" or as a reference for comparison.

Use sensitivity analysis or pathway modeling to evaluate surrogate data; if the results are sensitive to the surrogate values, some sampling and analysis is probably needed to verify these data.

Adapt Analogs

This approach involves extrapolating known data for one well-studied compound to predict the emissions for a compound with inadequate data. In this respect, it is another surrogate, but instead of using general geographic data for the same compound, it uses site-specific information for a different compound. An example might be the following: suppose that, in a given study area, airborne emissions of hexane are known, and are due to its use as a solvent in an industrial process. Pentane, a chemically similar compound, is an impurity in the solvent and its emissions are unknown. If the percentage impurity of pentane in the solvent is known, and the relative vapor pressures are known, the pentane emissions from the industry can be estimated to originate from the same point as the hexane emissions and at proportionately lower rates.

The use of analogous compounds is predicated on assumptions of similarities of use and chemical properties. Like the engineering estimates, mass balance calculations, and surrogate data, its use limits the confidence that can be placed on the data. The analytic tools discussed in the preceding section (sensitivity analysis/modeling) are helpful in evaluating the significance of the estimates generated by using analogs.

3.6 SYNTHESIZE AND INTERPRET DATA

The final subtask in the sources and emissions inventory is to synthesize and interpret the emissions data. The synthesis will generate a table for each source and discharge mode (based on receiving media) detailing the source locations, flows, concentrations, variability in discharge, and other pertinent information. Again, since the emissions data form the basis of most of the other exposure assessment and control strategy work, consult with the personnel involved in those tasks to ensure that the outputs from the source and emissions inventory are in a usable format.

Because the source and emissions inventory is the first task of the exposure assessment, the conclusions that can be drawn from it are, in a sense, preliminary. The final exposure conclusions cannot be reached until the pathways analysis, receptor and exposure route analysis, and final assessment are complete. Nevertheless, the source and emissions data alone can indicate some important trends.

For each of the toxics studied, aggregate the emissions from each type of source and discharge mode and compare them (e.g., 25% via industrial/ point sources, 30% via urban runoff, 10% via residential/air emissions, 25% via aqueous imports, and 10% via industrial/land-destined waste disposal). This kind of analysis can show where the greatest environmental loadings originate and what the primary discharge modes are. It may also be valuable for determining the effectiveness of existing regulations.

Similarly, the data can be aggregated by location of sources. Use this to identify 'hot spots' within the study area; the environmental pathways task will generate more complete information on 'hot spots'.

Data synthesis must involve a thorough description of all methods, assumptions, and equations used to generate the sources and emissions inventory.

Finally, the level of confidence in the data for each of the individual sources and emissions rates should be evaluated and tabulated. The level will vary depending on the adequacy of the data and the strength of the assumptions used to generate and manipulate the data base.

4. ENVIRONMENTAL PATHWAY ANALYSIS

4.1 OBJECTIVE AND SCOPE OF THIS SECTION

Environmental pathway analysis provides the link between quantification of source emissions and assessment of receptor exposure, by estimating the ambient concentrations of toxic substances in various environmental media. The objective of this section is to provide prospective users of the geographic methodology with generalized procedures and techniques for performing environmental pathway analyses. As such, this section provides general information for: (1) pathway analyses in specific environmental media (air, soil, water)--as well as between these media; (2) factors to be considered in trying to identify the most important pathways of toxics; (3) selection procedures for models and guidance for compiling the necessary data to drive these models; (4) guidance for interpretation of model output and model validation; and (5) additional issues that may arise during modeling efforts.

It is not the intent of this section to provide modeling details and material immediately applicable to perform a modeling effort. Rather, it is assumed that experienced environmental scientists will be responsible for mathematical modeling in a geographic study, and that they will be acquainted with the techniques presented below. Although it is not possible to provide a check list of "best" environmental modeling techniques covering all media, references are available (Bonazountas 1981) that present a thorough discussion of currently available models.

4.2 INTRODUCTION

A successful geographic study must quantify the relationship between chemical releases into the environment and the actual amounts of these chemicals to which humans and other biota are exposed. Only with detailed information as to pollutant concentrations in environmental media and the distribution of these concentrations can the issues of risks, human health, and environmental protection be addressed. Thus, the purpose of a pathways analysis is to describe the processes by which pollutants traverse through the environment, and to quantify the levels of pollutant at different points in each pathway.

Whether the concern is for human health or for environmental impact, the concentration of the chemical compounds at user-specified receptors or media of concern must be estimated. Concentration estimates can be obtained by: (1) knowing the distribution of releases of the material into the natural environment; (2) knowing the environmental conditions influencing the fate (transport/transformation) of the chemical compounds; (3) knowing the properties (physical/chemical) of the material; and (4) employing techniques for analyzing information gathered. These requirements are schematically shown in Figure 4-1.

Several techniques can be employed to investigate environmental pathways. Analytic sampling programs, for example, may be designed to measure actually occurring pollutant concentrations under a variety of conditions. These data may then be used both to estimate both actual levels, and to provide information about the processes and pathways that may be important at specific sites. However, sampling programs are costly to design and implement, and are also subject to biases due to the occurrence of unusual conditions during the actual time that samples are collected. Monitoring data from previous analytical work may also be used for these purposes, but such studies are subject to the same problems, with the additional limitation that these data are frequently incomplete, may be outdated, and are rarely extensive enough to provide a basis for evaluating an entire area.

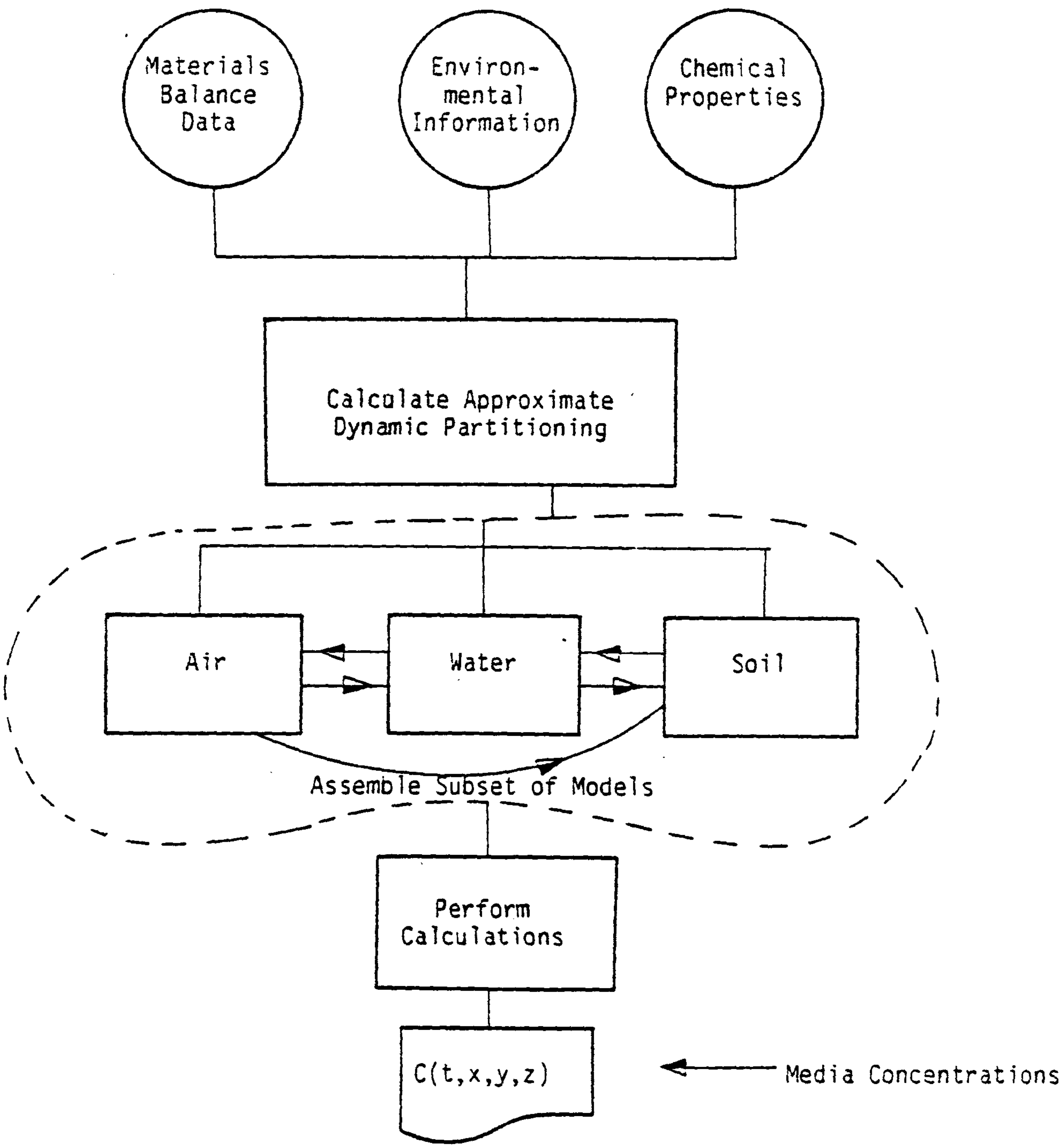


FIGURE 4-1 SYSTEM DESIGN SCHEMATIC FOR ENVIRONMENTAL MODELING

Mathematical computerized models of environmental processes are frequently used to generate information unavailable by other means, or to estimate data that are otherwise too costly to obtain. Models may have the added benefit of allowing the design of analytical programs that are more cost-effective, less subject to bias, and more attuned to the dynamics of a local area. Thus, environmental models are useful tools for identifying intermedia transfer mechanisms, generating necessary but unavailable data, and simulating a wide range of real and hypothetical environmental scenarios. Some important information, such as sensitivity of concentrations to changes in environmental parameters can also be obtained from the use of models. Mathematical modeling efforts are discussed in the Sections 4.3 and 4.4 below, and the incorporation of monitoring data is addressed in Section 4.5.

4.3 POTENTIAL PATHWAYS OF TOXICS

4.3.1 General Analytical Approach

Analysis of monitoring data may provide ambient concentration information for specific conditions, but to quantify the pollutant pathways in a region, environmental models are necessary. Thus, a pathway analysis usually involves choosing or adapting environmental models to be used to simulate pollutant behavior in the region of interest. Selecting the most appropriate model can be difficult, because there may be several different single models, mathematical expressions, or multimedia models to describe the same pathway. There is a tendency among scientists to use models they are "familiar" with, whether or not they are the most appropriate. Of course, in a given situation no single model is best, and sometimes it is difficult to differentiate the advantages and disadvantages of similar models. Users have to always exercise judgment and apply their valuable experience to model selection and application.

The two major stages in performing an environmental pathway analysis are:

(1) A rapid examination of background information relevant to the geographic specific study; and

(2) Performance of the quantitative analysis.

Stage 1--extends and amplifies the initial scan (see Section 2.5.2) and aims to:

(1a) identify potential (probable) pathways of toxics;

(1b) evaluate available data information of a specific region;

(1c) identify what receptors in the region might be affected or are of importance for further consideration; and

(1d) identify mathematical model candidates to estimate media concentrations.

Stage 2--quantitative analysis involves:

(2a) collection of monitoring and other site data;

(2b) definition of the important pathways in the region;

(2c) selection of models to simulate these pathways;

(2d) compilation of input data for the models;

(2e) performance of the simulations;

(2f) analysis of model output/results; and

(2g) output validation (with monitoring data) whenever feasible.

4.3.2 Examination of Background Information

The rapid examination of background information can save considerable time if carried out properly. This effort requires a strong interaction between team members of the study who: (1) perform the pollutant source inventory, and (2) perform the exposure analysis. Interaction with the first group may refine the modeler's understanding of spatial and temporal distributions of releases into the environment, and consequently will lead to an informed selection of single medium models. Interaction with the second group will lead to an environmental discretization (e.g., number and location of river segments) and consequently to the optimal implementation of the selected models (e.g., model output requested only at specific locations or receptors of importance, or at locations where monitoring data will be available).

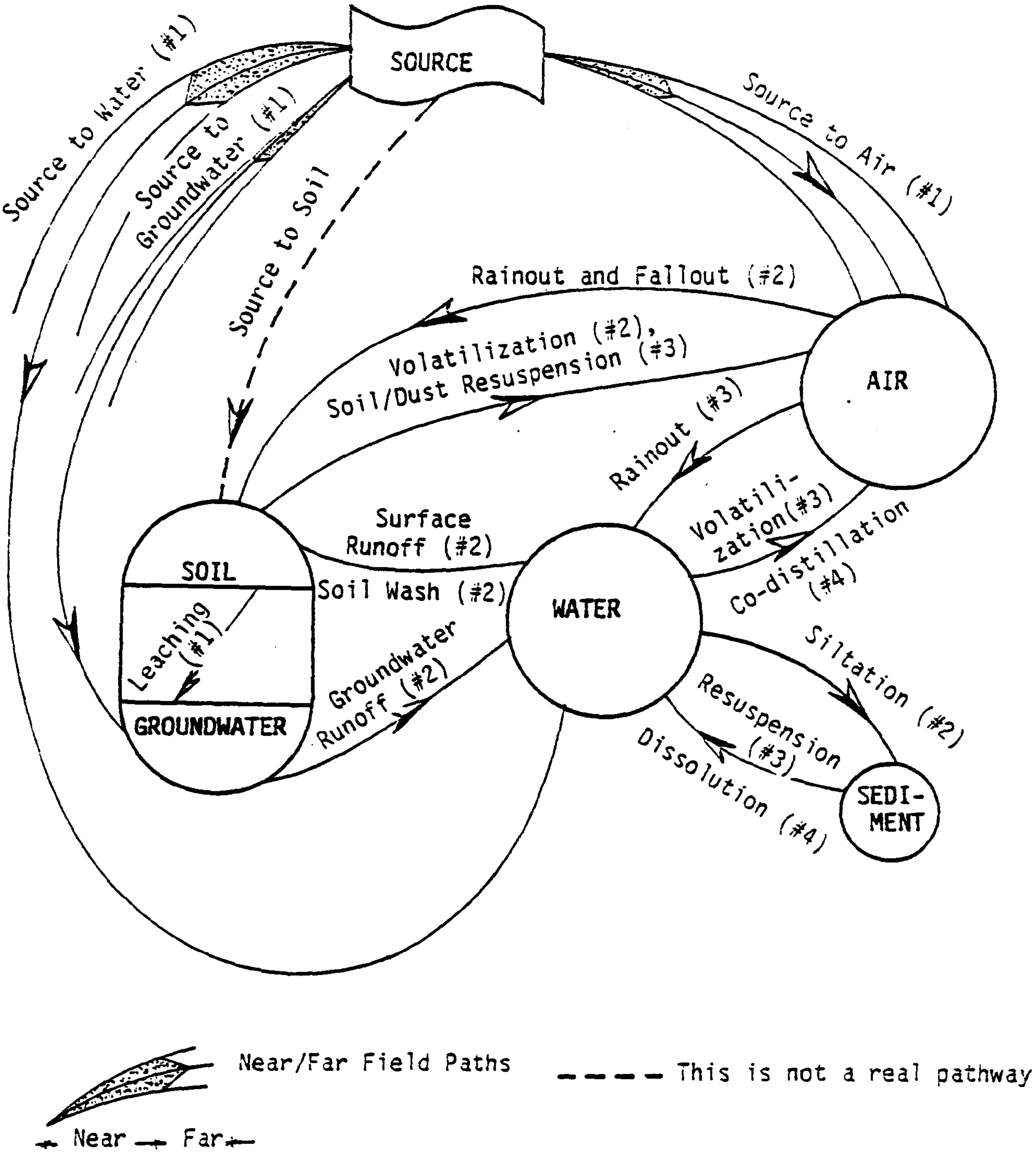
Coordination with the exposure group, regarding what receptor effects are likely to be of greatest concern, is also of importance during Stage I. Examples of receptor effects are toxicity to fish via the food chain in humans due to inhalation, chronic functional disorder in humans due to dermal absorption, lowered feeding rates in fish due to gill absorption, or mutagenic effects in humans due to drinking contaminated water. If the chemical substance is chosen for a fate analysis, it is most likely that some effect of concern has been already identified and can be used as guidance in constructing the optimal set of building blocks that will ultimately constitute the multimedia fate model.

Finally, considering the fate properties and potential receptor effects, during Stage 1, the user will gain a deeper understanding of the critical environmental pathways, and can establish priorities regarding Stage 2. For example, in dealing with a chemical whose main effect is toxicity to benthic organisms, the pathway leading from the sources through the air into the water and to the receptor would be a logical priority in establishing a model. Considering relative contributions of multiple release, modes, amounts, or dominant fate properties, certain pathways will be preferred to others in the rather large array of possible combinations. Flow charts or graphical diagrams become useful tools in identifying and establishing the pathway connections between sources and receptors needed for defining fate model approaches.

4.3.3 Quantitative Pathway Analysis

During Stage 2 the pathway analysis is performed. The situation immediately preceding calculations of concentration estimates is perhaps the most critical one of all: the choice of model logic used for each medium of interest and the designation of intermedia transfer processes. From the pathways diagram (Figure 4-2), the user can proceed to separately consider each medium and select the appropriate calculation technique or model that characterizes both the behavior in that medium and the transfers to other media from that medium. Judgment and experience must be exercised in this step in order to choose the appropriate time and space scales for the problem. A possible complication might be that chemical transformations may effectively terminate the pathway within a specific medium. Preliminary half-life estimates for transfer and transformation, and a comparison among them will adequately serve the purpose of indicating which fate properties are important to consider.

The following paragraphs present five hypothetical examples (Aravamudan et al. 1980) intended to illustrate the thinking required to analyze and model the fate of a chemical. Examples deal with:



#1 Direct discharge pathways.

#2-4 Intermedia discharge pathways (primary, secondary, potential).

Degradation of substances can take place in any compartment.

Out-of and into basin transfers are not shown.

Source: Bonazountas 1981

FIGURE 4-2 ENVIRONMENTAL PATHWAYS OF TOXIC SUBSTANCES

(1) Point source atmospheric emissions;
(2) Area source atmospheric emissions;
(3) Point source water discharges (low vapor pressure);
(4) Point source water discharges (rapid hydrolysis);
(5) Non-point source water discharges (runoff source).

(1) First consider the case where pollutant A is primarily emitted from a combustion point sources into the air. Upon reviewing the properties of A, we find that it has a relatively low vapor pressure and a low solubility. The chief target of concern is human receptors exposed through either the inhalation or ingestion pathways. The reasoning that we go through leads us to two primary pathways: (a) direct inhalation from the air of the material which has adsorbed onto aerosol particles; and (b) an appearance of material on soil or sediments by way of deposition to the earth surface. The deposition is followed by runoff of particles to which the material is adsorbed, in the case of terrestrial deposition. Direct washout eventually leads through aquatic pathways. In both cases, the material ends up in sediments.

Microorganisms are known to bioconcentrate the material through food chains leading to fish that are part of the human diet. The environmental simulation will include a variety of climatologic conditions in the region for point source plume calculations of non-reactive pollutants. The nonreactive designation is obtained by comparing the half-life due to photo-oxidation with the time required for adsorption on aerosol particles and deposition. If physical fate mechanisms dominate, then the material is assumed to be nonreactive. The mathematical models for water would be the homogeneous well-mixed cell models because of the wide distribution of input from the various air to surface deposition processes and the long time scales of interest.

(2) As a second example, consider an area source emission into the atmosphere of some solvent material (pollutant B) having a modest vapor pressure and a reasonably high value of aqueous solubility. The area source associates the material with an urban plume. This indicates that the air model to be used would be a widely dispersed source model that gives a plume spreading rapidly up to the atmospheric mixing height but spreading horizontally only at a rate dictated by turbulence in the direction transverse to the wind. Pollutant B is assumed to have known serious effects only on aquatic ecosystems. Since the discharges are primarily into the atmosphere, the mechanism of transfer from the plume to the surface must be part of the fate model.

Again, the pervasive use of the material requires that a range of atmospheric environmental conditions be employed. Both dry deposition and rainout will be considered as air to surface transfer mechanisms because the material has a reasonably high solubility. The Henry's Law constant can be used to determine an upper concentration limit in the rain water. The rainfall rate along with runoff quantities downwind of an urban area are used to establish the material in the water. Concentrations thereby estimated provide an input to exposure calculations.

(3) Another example may be water discharges from point sources. The assumed pollutant C has a low vapor pressure and moderate solubility. It has a relatively high partition coefficient between the organic material and sediments. The main concern regarding this pollutant is the concentration of its residues in crops that are at the base of the human

food chain. For discharges into aquatic environments, variable stream flow conditions (high, low, medium) have to be considered. The stream water may be used as irrigation water and, therefore, biota compartments (initially crops) will be exposed to the material. Bioconcentration factors for agricultural crops used for cattle feed and subsequently in meat products give the ultimate concentrations needed.

(4) Consider pollutant D that is primarily discharged into the water. An overwhelming fate property of this material is its rapid hydrolysis. The point source discharge calculation with a half-life appropriate to the hydrolysis superimposed on it is an appropriate method for estimating the zone of influence in this material. If human ingestion through drinking water is the pathway of concern, then the range of influence between discharges and inlets to drinking water treatment facilities becomes a key parameter in determining whether the fate calculation is even appropriate. Various scenarios (see Exposure Analysis section; Chapter 5) for these site specific conditions are drawn from situations where the material is apt to be discharged. Assessments are made based on these data.

(5) As a final example, consider pollutant E that is primarily discharged into the water from a variety of runoff sources. A chemical that is disposed of on land, or is distributed over land by immediate spreading, directs the user to the soil compartment modeling section of this chapter (see Section 4.4.4; Soil Compartment Modeling) and calculations proceed to determine relative quantities of material in soil moisture, surface runoff, groundwater runoff and the soil itself.

Either the full operation of the analytical models described in Section 4.4 of this chapter or simple equilibrium partitioning may be employed to arrive at concentration or transport estimates. If the main target receptor of the material is a terrestrial ecosystem, then biotic considerations become of importance by providing, for example, an entry point to a food chain for the material. Also, the possibility of biodegradation in the soil or in the food chain at some point must be considered. Losses due to vaporization from the soil and to leaching must be introduced into the model calculations in order to arrive at an appropriate mass balance of material.

4.4 MATHEMATICAL MODELING

4.4.1 General Overview

The following paragraphs describe the objectives, structure and intended use of the three major model categories (air, soil, water). Coordinating the brief discussion of sample chemical assessment given above with these brief explanations will provide the user with a perspective on the optimal application of the various single medium or multimedia models. Two other summaries briefly describe the materials balance aspect of a fate analysis (Section 4.4.6.2) and the logic by which an initial approach to the analysis may be determined (Section 4.4.6.1).

Previous modeling efforts have focused upon two distinct modeling areas: (1) single medium pathway (or fate) models; and (2) multimedia pathway models, both applicable to a variety of environmental conditions and types of pollutants. Often, however, their applicability is limited, due to data availability, complex physical boundary conditions or insufficient mathematical description of processes (physical/chemical) involved. Multimedia models have been constructed in the past by sequentially linking (interfacing) single medium models and using other equations to describe transfers between the media.

Generalized discussions and information regarding environmental modeling can be found in numerous reports or publications (Miller 1978) and other exposure assessment documents (EPA 1980). EPA's Catalogue of Environmental Models (EPA/MIBS 1979) is a recent comprehensive compilation of selected models for water quality, surface runoff, soil quality, air quality, and economic analysis.

Only a short description of the types of models available for each environmental medium (air, water, soil; Figure 4-2) with a few examples of each type are presented in this section, since a comprehensive "Multi-media Environmental Modeling Background/Catalogue" (Bonazountas 1981) contains detailed state-of-the-art information.

4.4.2 Air Compartment Modeling

Air modeling efforts encompass both near-field and far-field investigations (Figure 4-2). Briefly, models of urban scale are the most advanced of the air quality models. They model the dispersion process for area and point sources, for reactive and non-reactive gases. Some allow for variations in meteorology; most are limited to noncomplex terrain. These models are now being validated with field data, and efforts are being made to simplify the required data input, depending on the application, and to assess the models' accuracy and costs (Miller 1978). A considerable amount of air modeling effort is being conducted at the EPA Environmental Sciences Research Laboratory, Research Triangle Park, North Carolina.

There exists a library of EPA-developed computer programs which all contain a basic source-oriented atmospheric dispersion model. The features and assumptions of these programs should be critically examined with respect to the needs of the geographic study. This library of programs continues to grow and the capabilities of more recent additions to the set may be flexible enough to treat source-to-air and air-to-air pathways assessment for pollutants. Table 4-1 identifies selected programs of the library and their features. In a geographically bounded exposure assessment it may be necessary to analyze several toxic substances and/or several modes of exposure for one or more substances, still within the framework of the air pathway. Thus, it may be necessary to select and apply more than one of the algorithms listed in Table 4-1.

Air-to-surface pathway modeling can be performed either as part of the air compartment simulation or separately. Additional information is given by the "Multi-media Environmental Catalogue" (Bonazountas 1981).

Of all the compartmental simulations, the air compartment is probably the least well defined of all because of the lack of distinct boundaries. In attempting to postulate a well-mixed description for chemical transport and transformation in the air, one must define boundaries that take account of advection and diffusion. Consequently, the air compartment may not be a simple box, but rather a time-variable control surface with permeable boundaries. Fortunately, these difficulties are somewhat offset by the extensive inventory of air quality models. For example, plume formulations and vertical diffusion solutions may provide guides for defining the growth and motion of an air compartment. Its size and variability will depend upon the geometry of the source array and the chemical lifetime of the material in question (Aravamudan et al. 1980).

The scope of work when performing an air compartment simulation begins with an identification of the source characteristics (line source, point source, area source, or urban area source), and proceeds with the location and time dependence of the release mode. Physical characteristics of the source such as mass flow and buoyancy are ob-

Table 4-1

FEATURES OF OFF-THE-SHELF EPA AIR MODELS FOR TOXIC SUBSTANCE EXPOSURE ASSESSMENTS*

	RAM	ISC	CRSTER	PAL	CDM	HIWAY
Source	point, area	point, area, line, volume	point	point, area, line	point, area	line
Source Dynamics	vary rate hourly	many options	vary monthly average	vary hourly	day/night	none
Spatial Range	near-field & far-field	near-field & far-field	far-field	near-field	near-field & far-field	near-field
Temporal Range	hours to 1 year	hours to 1 year	hours to 1 year	limited sequence of hours	seasonal/ annual	limited sequence of hours
Removal Mechanisms						
- chemical	first-order	first-order	first-order	none	first-order	none
- physical	none	dry deposition of particulate	none	none	none	none
					none	elevated or cut roadway segments
Special site Considerations	elevated terrain impacts	elevated terrain impacts	elevated terrain impacts	none		

*This list of models is not comprehensive: these few were selected on the basis of their range of features, their flexibility for current air quality regulatory applications, and appropriateness of model outputs.

tained from site specific information. If the material is chemically reactive in the air, appropriate rate expressions have to be obtained from the literature.

Another class of input information to the air compartment includes meteorological and topographical conditions which will affect the advection and diffusion of the pollutant. This includes an examination of the temperature data, wind velocity data, and the stability classification of the atmosphere. Gross topographic features describing the type of terrain that may influence the conditions of the atmospheric boundary layer are also specified. Table 4-2 lists input data categories of an air modeling effort.

Meteorological data are archived at the National Climatic Center in Asheville, North Carolina. Available data sources need to be reviewed to determine which station has collected the most representative data to input into the models. If none of the National Weather Service stations adequately represent conditions within the study area, private, government or industrial data sources should be reviewed to consider the suitability of these sources. Monitoring within the study area is another possibility; but, this option can be quite costly.

Some important issues to consider in selecting the most representative meteorological data base are:

- Topographic effects, such as valley flows and water/land interfaces should be considered such that wind flow and stability are representative of the study area.

- If National Weather Service data are used to estimate stability, caution must be used if local influences would result in substantially different stability conditions than those predicted solely from insolation and

Table 4-2

INPUT DATA CATEGORIES OF AIR COMPARTMENT SIMULATIONS

(1) Source and Pollutant Characteristics

* source type (point, line, area, urban)
* source location (x,y coordinates; r,θ coordinates)
* pollutant type (reactive, non-reactive, gaseous, particulate, buoyancy of effluent)
* release mode (continuous, instantaneous)

(2) Meteorologic and Topographic Characteristics

* atmospheric stability classification
* temperature, wind velocity
* cross topographic features

(3) Other Data

* dispersion data
* control parameters (output), type of simulation
* time resolution (1 hr, 24 hrs, average, extremes)

wind speed. Topographic anomalies, urban effects, differences in surface heat capacities, and other factors can influence stability, but are not accounted for by the Pasquill-Turner stability classification system.

- Wind sensors associated with the collection of the data base should be located such that local influences from building wake effects, trees, and terrain irregularities do not unduly modify flow.

  The height of the wind sensors should be representative of the layer into which the pollutants will be dispersed. If the heights are significantly different, corrections based upon wind profile considerations should be applied during processing of the data.

- The quality assurance of the data set, based upon calibration documentation and data review, is an important factor regarding its acceptability.

- A long-term data set (i.e., greater than five years) is preferable to a short-term data set because of year-to-year variation of meteorological parameters.

4.4.3 Soil Compartment Modeling

Soil and groundwater models are used to model "source-to-soil," "soil-to-groundwater," "groundwater-to-water," and "soil-to-water" pathways. The variety and complexity of mathematical models (i.e., set of equations) used in soil/groundwater application have increased dramatically during the last ten years. The proliferation of models is often bewildering to both the scientist who is trying to keep up with the research literature and to the user who is trying to find the best model. Ironically, although the number of model types is large, only a few basic processes can be modeled, so that the large number of apparently different models are the results of a variety of simplifying assumptions used to reduce the general set of equations to a solvable set.

Three types of "soil" models can apply to various parts of the soil environment: (1) "unsaturated soil zone" models that simulate conditions of a soil zone profile extending between the ground surface and the groundwater table, and may include runoff and volatilization processes; the Seasonal Soil Compartment model (SESOIL) is a model of this type; (2) "groundwater" models that generally simulate the flow and quality of specific groundwater aquifers; and (3) "watershed" models that focus on the interactions at the soil surface such as overland flow (runoff), and sediment transport and quality. The Agricultural Runoff Management (ARM) model is of this type. These model types can and do overlap.

The choice of a soil model requires finding the best compromise between needed level of sophistication, available data, and needs and resources (computer, time, and budget) of the project. Tables 4-3 through 4-6 present some of the available models for various aspects (unsaturated, saturated, unsaturated/saturated, watershed) of soil modeling, whereas the "Multi-media Modeling Environmental Catalogue" (Bonazountas 1981) provides in depth discussions for the various pathways of a soil compartment.

Once the soil models have been chosen, the data for specific model runs must be gathered. The actual data required will be specific to the model used, and the pathways involved. However, some general data categories can be identified such as source data, climatological data, geographical data, particulate transport data, and biological data. Table 4-7 presents some parameters associated with each category. Table 4-8 presents some sources of data mentioned in Table 4-7.

TABLE 4-3

PARTIAL LIST OF UNSATURATED (U) SOIL ZONE POLLUTANT TRANSPORT MODELS

Model Number	Principal Investigator	Model[1] Dimensionality	Solution[2] Technique	Type of[3] Flow	Type of[4] Soil	Type of[5] Chemical Interactions	Application/Comments
U-1	King and Hanks (1973, 1975)	1D	FDM	Tr	-	Ad, De, Ce	Applied to irrigation return flow quality studies. Includes plant root uptake of water.
U-2	Smajstrala et al. (1975)	1D	0	Tr	-	-	Miscible displacement in soils.
U-3	Bresler (1975)	2D,C	FDM	Tr	-	-	Describes two-dimensional transport of solutes under a trickle source.
U-4							
U-4	van Genuchten and Pinder (1977)	1D	FEM	Tr	L	Ad, De, Ce	Modeling of leachate and soil interactions in an aquifer.
U-5	Hildebrand and Himmelbau (1977); Hildebrand (1975)	1D	FDM	Tr	-	-	Transport of nitrate in a sand column
U-6	Selim et al. (1976a)	1D	FDM	Tr	-	Ad	Applied to transport of 2,4-D in soils.
U-7	Ungs et al. (1976)	1D	FDM	Tr	-	Ad, De	Compared results with observed field data on chloride transport during infiltration.
U-8	Selim et al. (1977)	1D	FDM	St	L	Ad	Applied to Cl and 2,4-D movement in two-layered soil column
U-9	Gureghian et al. (1977)	1D	FDM	Tr	L	Ad, De, Ce	Simulation of pollutant transport in Long Island, N.Y.
U-10	Shah et al. (1975)	1D	FDM	St	L	Ad	Applied to phosphorus transport in soils; assumes constand dispersion coefficient and kinetic model for phosphorus adsorption.
U-11	Bonazountas et al. (1979)	1D	FDM	Tr	L	Ad, De	Describes vertical solute transport in soils. Can be linked to FD or FE models.
U-12	Bonazountas (1980)	3D	0	St	-	Ad, De, 0	A seasonal soil model, SESOIL.

1) 1D = one-dimensional; 2D = two-dimensional; 3D = three-dimensional; A = Areal (2D only); C = Cross-sectional (2D only)

2) FDM = Finite Differences Method; FEM = Finite Element Method; 0 = Other

3) Tr = Transient; St = Steady-state

4) L = Layered

5) Ad = adsorption; Ce = cation exchange (multi-ion transport); De = decay

TABLE 4-4

PARTIAL LIST OF SATURATED (S) SOIL ZONE (GROUNDWATER) POLLUTANT TRANSPORT MODELS*

Model Model Number	Principal Investigation	Model Dimensionality[1]	Solution Technique[2]	Type of Plan[3]	Type of Soil[4]	Type of Chemical Interactions[5]	Application/Comments
S-1	Robertson (1974); Robertson and Barraclough (1973)	2D,A	C	Tr	An	Ad, De	Transport of industrial and low-level radioactive wastes into the Snake River Plain aquifer, Idaho. Simulated 20 year history of pollution.
S-2	Ahlstrom and Baca	2D,A	0	St/Tr	An	Ad, Ce	Considers adsorption and exchange of several macro- and micro-ions.
S-3	Thoms et al. (1977); Martinez et al. (1975)	2D,A	FEM	St	-	Ad, De	Describes groundwater pollution from salt dome leachates.
S-4	Robertson (1975)	2/3D 2/3D	0 0	Tr Tr	An,L An,L	Ad, De	Three-segment model for flow, including ability to simulate perched water in the unsaturated zone.
S-5	Konikow (1976)	2D,A	0	St			Simulated 30 year history of groundwater pollution by chloride from an unlined disposal pond into the underlying alluvial aquifer.
S-6	Helweg and Labdle	2D,A	0	Tr	An	-	Adapted version of S-9; used as a cost-effective salinity management technique for stream-aquifer systems.
S-7	Pickens and Lennox (1976)	2D,C	FEM	St	L,An	Ad	Contaminant transport from a hypothetical landfill.
S-8	Schwartz (1975, 1977)	2D,C	FEM	St	An	Ad, Ce, De	Hypothetical study of subsurface pollution by radioactive wastes (1975); model analysis of a proposed waste-management site (1977).
S-9	Konikow and Bredehoeft (1974a, b)	2D,A	0	Tr	An	Ad, De	Used calibrated model to evaluate effects of different irrigation practices on salinity changes in an alluvial stream-aquifer system.
S-10	Guregnian and Cleary (1977)	3D	FEM	St	An	Ad, De	Applied to an existing landfill on Long Island
S-11	Besbes et al. (1976)	2/3D,A	FD	Tr	L	-	A real model for multilayered aquifer system; predicted concentration changes after dam construction in the Kairouan Plain, Tunesia
S-12	Fried (1971, 1975); Fried and Ungemach (1971)	2D,A	FD	Tr	-	-	Flow part based on Boussinesq equation; describes pollution by NaCl from large salt dumps into alluvial aquifer in Northeastern France.
S-13	Pinder (1978)	2D,A	FEM	Tr	An	Ad	Applied to hazardous waste disposal sites, to estimate groundwater contamination and plume development.

*See footnotes, Table 4-5

Source: Bonazountas 1981

TABLE 4-5

PARTIAL LIST OF UNSATURATED/SATURATED (US) SOIL ZONE POLLUTANT TRANSPORT MODELS

Model Number	Principal Investigation	Model[1)] Dimensionality	Solution[2)] Technique	Type of[3)] Plan	Type of[4)] Soil	Type of[5)] Chemical Interactions	Application/Comments
US-1	Perez *et al*. (1974)	2D,C	FDM	Tr	L	-	Groundwater pollution from agricultural sources.
US-2	Elzy *et al*. (1974)	2D,C	O	Tr	-	Ad, De	Contaminant movement from a landfill.
US-3	Sykes (1975)	2D,C	FEM	St	L,An	-	Contaminant movement from a landfill.
US-4	Duguid and Reeves (1976, 1977)	2D,C	FEM	Tr	L,An	Ad, De	Transport of radionuclides from a waste-disposal site. Might be applied to waste sites.
US-5	Segol (1976, 1977)	2D,3D	FEM	Tr	L,An	-	Not applied yet.
US-6	Van Genuchten *et al*. (1977)	2D,C	FEM	Tr	L,An	Ad, De	Leachate movement from a hypothetical landfill.

1) 1D = one-dimensional; 2D = two-dimensional; 3D = three dimensional; A = Areal (2D only); C = Cross-sectional (2D only)

2) A = Analytical; FDM = Finite Differences Method; FEM = Finite Element Method; O = Other

3) Tr = Transient; St = Steady-state

4) L = Layered; An = anisotropic

5) Ad - adsorption; Ce = cation exchange (multi-ion transport), De = decay

Source: Bonazountas 1981

TABLE 4-6

PARTIAL LIST OF "WATERSHED" MODELS

Model Acronym	Carrier Vehicles	Exposure Routes	Basis and Summary Features
GWMTM1	Ground Water	All determinable from knowledge of concentration	Based on convective-dispersive mass transport equation modified for 1st order decay. 1-dimensional treatment. Surface concentration can be constant or exponentially varying. Vertical seepage constant. Soil saturated or unsaturated.
GWMTM2	Ground Water	All determinable from knowledge of concentration	Describes concentration distribution in 2 underground dimensions. Advection and dispersion in 2 dimensions with 1st order decay and an exponentially decaying Gaussian boundary condition. Useful for sanitary landfills, wastewater lagoons, and chemical dumps.
EPAURA	Runoff Water	All determinable from knowledge of concentration	Assumes accumulated pollutants are all carried off in rainfall on an area of impervious surface.
EPARRB	Runoff Water	All determinable from knowledge of concentration	Assumes all rural areas have slope percentages allowing erosion to take place. Calculates delivered sediment to a water body based on the universal soil loss equation. Pollutant loads are outputed.

TABLE 4-6 (continued)

Model Acronym	Carrier Vehicles	Exposure Routes	Basis and Summary Features
NPS	Runoff Water	All determinable from knowledge of concentration	Used to estimate nonpoint source pollutant loads in urban and rural settings.
AGRUN	Runoff Water	All determinable from knowledge of concentration	Simulates hydrology and channel pollutant loads for agricultural watersheds. Uses the universal soil loss equation and Horton's equation to compute infiltration rates. Requires specification of soil parameters.
ARM-II	Runoff Water	All determinable from knowledge of concentration	Mass balance. Assumes all runoff water from locations in the watershed. Pollutant transformations are approximated by a series of 1st rate expressions. Arrhenius equation used to adjust rates to different temperatures. Partitioning between phases assumed to be instantaneous.
HSPF	Runoff Water	All determinable from knowledge of concentration	Mass balance. Assumes all runoff water from locations in the watershed. Pollutant transformations are approximated by a series of 1st rate expressions. Arrhenius equation used to adjust rates to different temperatures. Partitioning between phases assumed to be instantaneous. Water body simulations.

TABLE 4-6 (continued)

Model Acronym	Carrier Vehicles	Exposure Routes	Basis and Summary Features
SESOIL	Runoff Sediment	All determinable from knowledge of concentration	Statistical seasonal (month, year) user specified simulation, stochastic poisson and gamma distributed functions. In-depth chemistry, analysis, applicable to both organic and inorganic compounds.

Source: Bonazountas (1981).

Table 4-7

SOIL COMPARTMENT ENVIRONMENTAL PARAMETERS
(EXPOSURE PATHWAY MATRIX)

PARAMETER (Variables)	EXPOSURE MEDIUM		
	Soil and Groundwater	Surface Water	Air
• CLIMATE	X	X	X
Evapotranspiration			
Temperature			
Latitude			
Sunlight			
Plant Cover			
Humidity			
Cloud Cover			
Wind			
Precipitation			
• SOIL	X	X	
Porosity			
Density			
Hydraulic conductivity			
Permeability			
Adsorption capacity			
Organic carbon content			
Clay content			
• GEOGRAPHY	X	X	X
Slope			
Surface storage			
Terrain			
Receptor locations			
• PARTICLE TRANSPORT		X	X
Wind			
Flood flow			

Table 4-7 (Continued)

PARAMETER (Variables)	EXPOSURE MEDIUM		
	Soil and Groundwater	Surface Water	Air
• BIOLOGICAL ACTIVITY		X	X
Plant coverage Plant types Bioconcentration (both by plants & animals) Biological degradation			
• SOURCES	X	X	X
Emission rates Release mechanisms Patterns of operation (continuous, batch) Locations			

Table 4-8

DATA SOURCES FOR SOIL COMPARTMENT ENVIRONMENTAL PATHWAY ANALYSES

Climatological Data:

National Oceanographic and Atmospheric Administration (NOAA) Reports

Soil Data:

United States Geological Survey (USGS) Reports
United States Army Corps of Engineer Reports
Federal and Regional Agricultural Agencies
Landfill and Industrial Operators

Geography Data:

USGS Maps and Reports
Census Bureau Data

Particle Transport:

USGS Surveys
Army Corps of Engineers Reports

Biological Activity:

Agricultural Agencies
Environmental Agencies
Universities

Sources:

Industry Representatives and Operators
Regional Discharge Permit Boards
Environmental Agencies

4.4.4 Water Compartment Modeling

Water quality models describe transport and transformation of substances from point discharges and non-point sources, including urban and non-urban runoff. Many models predict concentration levels for water quality parameters such as dissolved oxygen, nitrogen, phosphorous, and pH; others can predict concentration levels of certain chemicals in the water body. Most of the models can account only for organic compounds (transport, dispersion), others can account for both organic and inorganic (metal) compounds.

Models are structured according to the physical shape of the waterbody (lake, river, estuary) and according to the type of discharges (point source, non-point source). A few of these models are mathematically structured around a mass balance equation describing inflow, outflow and transformation of the chemicals in a given water volume. Others are based on partial differential equations describing flow and mass transport in fluid, the latter being from mass balances of a given element.

Water compartment models are applicable to rivers, ponds, lakes, estuaries and coastal nearshore waters. A simulation should be capable of providing estimates of either time-dependent or quasi-steady-state aqueous concentrations. The compartment size and time scales are established by the flow characteristics, the chemical degradation processes, the discharge characteristics, the inter-compartmental transfer times for each chemical/waterbody configuration, the exposure assessment requirements, etc. Pollution input from other compartments (e.g., air, soil, upstream water compartment) and pollutant transfer to other downstream or adjacent compartments are part of a water compartment modeling effort.

Two fundamental situations give rise to the family of water fate models. One is a well-mixed water body, either in place (e.g., pond), or in motion (e.g., segment of a stream undergoing time-variable boundary conditions). The other relates to the problem of non-uniform concentration fields associated with point sources of discharge, and results in the selection of a near-field (i.e., plume) or a far-field model.

Various models and additional information are presented in the "Multimedia Environmental Modeling Background/Catalogue" (Bonazountas 1981) and in Table 4-9.

In general, water models that are strong in physics (i.e., hydrodynamic models) are weak in chemistry (i.e., water compartment models) and vice versa. The choice of which model type to use depends on the objective of the study. A selected water quality model should in general be capable of:

(1) Simulating all the important aquatic environments (rivers, estuaries, pools) within the region of study.

(2) Accounting for adsorption of pollutants on abiotic surfaces, particulate matter and bed sediment.

(3) Treating movement of dissolved pollutants in water, as well as movement of pollutant associated with sediment.

(4) Handling water-sediment exchange.

(5) Accounting for important loss processes, both transport and transformation (e.g., volatilization, hydrolysis, etc.).

Two useful water models, known for their diversity, strength in chemistry and physics, and recent applicability are:

TABLE 4-9

PARTIAL LIST OF WATER-BODY MODELS

Model Acronym	Carrier Vehicles	Exposure Routes	Basis and Summary Features
EXPLORE-1	Water	All determinable from knowledge of concentration	Handles 1-dimensional flow in streams and rivers, 2-dimensional flow in shallow lakes and estuaries. Capable of handling constant or time-varying point or diffuse sources of substances.
MS CLEANER	Water	All determinable from knowledge of concentration	Sophisticated model with use in determining bioaccumulation of toxic substances.
DIURNAL	Water	All determinable from knowledge of concentration	Used to predict diurnal fluctuations during periodic steady state conditions. Useful when algal oxygen production is related to concentration of effective agent.
FEDBAK03	Water	All determinable from knowledge of concentration	Mass balance. Handles consecutive reactions and 1st order kinetics. Assumes that steady state conditions apply.
PLUME	Water	All determinable from knowledge of concentration	Considers only mixing and dilution with no water flow in a steady state stratified environment. 3-dimensional output. Provides concentration data along plume centerline.

TABLE 4-9 (continued)

Model Acronym	Carrier Vehicles	Exposure Routes	Basis and Summary Features
QUAL-II	Water	All determinable from knowledge of concentration	Simulates dynamic behavior of constituents subject to dispersion, flow, nutrient cycles, and algal growth. 1-dimensional for networks. Considers 1st order decay. Only point discharges and constant inflows are considered. Instantaneous mixing is assumed.
SEM	Water	All determinable from knowledge of concentration	Handles only point source inputs to streams. rivers, and shallow non-stratified lakes. 1st order decay. Simulates dilution, advection, and temperature effects. 1-dimensional. Considers uncoupled chemical reactions. Suitable for hand calculator.
ES001	Water	All determinable from knowledge of concentration	Mass balance. Can be used for sequential reactions of two substances having 1st order kinetics. Tidally averaged, steady state model. Suitable for complex water networks (100 junctions, 50-100 sections).
DEM	Water	All determinable from knowledge of concentration	Real-time, link node model simulating unsteady tidal flow and dispersion in an estuary. Two-dimensional flow. Hydraulic and quality (pollutant concentration) model components. Mass balance checks at each junction. Predicts time varying concentrations.

TABLE 4-9 (continued)

Model Acronym	Carrier Vehicles	Exposure Routes	Basis and Summary Features
TTM	Water	All determinable from knowledge of concentration	Derivative model of DEM. Handles up to 4 consitituents with coupled or non-coupled reactions with 1st order decay. Used for networks (300 junctions, 300 channels).
HARO3	Water	All determinable from knowledge of concentration	Mass balance. Multidimensional, steady state model for two reacting substances. Handles 1st order kinetics. Incorporates convective-diffusive mass transport with source and decay terms.
EH	Water	All determinable from knowledge of concentration	Simulates near shore currents and exchange processes. Sophisticated treatment of dispersion, advection, and dynamic plumes.
REDEQL	Water	All determinable from knowledge of concentration	Computes equilibria for up to 20 metals and 30 anions in a system. Includes complexation, precipitation, redox, and pH dependent reactions.
RECEIV-II	Water	All determinable from knowledge of concentration	Two-dimensional model representing advection, dispersion and dilution. Used on networks. Can simulate coupled and non-coupled chemical reactions. 1st order decay considered. Assumes instantaneous mixing.

TABLE 4-9 (continued)

Model Acronym	Carrier Vehicles	Exposure Routes	Basis and Summary Features
EXAMS	Water	All determinable from knowledge of concentration	A water body compartment model, providing user specified flexibility in application. Strong in chemistry of organic compounds. No metal chemistry, no sediment transportation routines.

Sources: EPA/MIBS (1981); Bonazountas (1981).

(1) EXAMS (Exposure Analysis Modeling System); a water compartment model of EPA (1980), Athens Research Laboratory; and

(2) EXPLORE, a river basin water quality model developed by Battelle Memorial Institute.

Basic parameters for the nation's water bodies to run water quality models, such as pH, DO, etc, are reported in STORET, NASQUAN, USGS and EPA data bases (see Section 4.5.4).

4.4.5 Multimedia Modeling

An overall model for the environmental fate of a substance in the air, soil, subsoil/groundwater, water, and biotic environment of an area can be constructed by sequentially interfacing single medium models, such as those described in the previous sections. However, the usefulness of such a "super-model" might be questioned, not because of the capability of this model to predict overall fate of pollutants in the environment, but because no "general" model can be developed that can account for all environments and all pollutants. Limitations of multimedia models are mainly due to the limitations of single medium models available and to the mathematics of interfacing those models.

Multimedia environmental problems are receiving increasing attention as more of them are recognized. A few multimedia models for assessing such problems are available; all of them focused on pollutant fate in a triple environment: air-watershed-water body. A few of the existing models are presented in Table 4-10. Their applicability, limitations, and deficiencies are briefly described in the "Multi-Media Environmental Modeling Background/Catalogue (Bonazountas 1981).

Table 4-10

PARTIAL LIST OF MULTI-MEDIA MODELS

Acronym	Major Features	Description
UTM	"air-watershed-stream" simulations	The focus of the Universal Transport Model (UTM) has been on watershed phenomena that are important to trace contaminant mobility and pathways including atmospheric dispersion, deposition on land, entrainment and erosion in overland flow, movement and exchange of soluble chemical species with a moisture flux through the soil matrix, transport in the stream channel, and exchange with the stream sediment.
CMRA	"Overland Flow - Stream" contaminant transport	The Chemical Migration and Risk Assessment (CMRA) methodology combines off-the-shelf overland and in-stream transport models, statistical analysis routines, and risk assessment procedures into a single system, in order to predict the probability of acute and chronic impact on aquatic biota.
ALWAS	"Air-watershed-water" contaminant transport	The objective of this study was similar to the objective of the UTM model, and theoretically there is no conceptual difference between the UTM and the ALWAS model. Both treat atmospheric emissions, surface runoff and stream quality. The scope of work, however, of ALWAS focuses in interfacing an atmospheric model, the nonpoint source (NPS watershed model and the exposure assessment modeling system (EXAMS) model into one single multi-media package. In addition, ALWAS provide more accurate insight into the deposition processes from air-to-surface (water, land).
TOHM	"Air-watershed-water" metal transport	The environmental Transport Model of Heavy Metals (TOHM) is tailored to heavy metals, stack emissions of coal-fired electric utilities, and semi-arid climate reaches. The development of TOHM consisted of interfacing an atmospheric model, and a soil chemistry model.

Table 4-10 (Continued)

Acronym	Major Features	Description
CONCEPTUAL	"Pesticide"-in environment	A conceptual model for the movement of pesitcides through the environment developed by the EPA's alternative chemical program. The study presents a conceptual model for the movement and disposition of pesticides in the environment. A multi-media model is built up conceptually from simple modules representing basic processes and components of air, soil, and water.
	Environmental Partitioning Model	An Environmental Partitioning Model for Risk Assessment of Chemicals, encompassing air, soil, water, biotic and partitioning logics. Unpublished document (Aravamudan *et al*. 1980).

Source: Bonazountas (1981).

By counting the limited number of individual models presented in the previous sections, for all potential pathways, it is easy to realize that a missing feature from a key model (e.g., volatilization from ARM) might be an adequate reason for a basic modeling package to require modifications. Furthermore, as time progresses, new models which are either directly applicable or applicable after modification will become available. Such new models will replace older packages and may simultaneously facilitate and improve simulations. Therefore, the design of a multimedia package can never be considered as "final"; rather it has to be regarded as continuously evolving. A multimedia model design interfacing (1) EXAMS, (2) SERATRA, (3) SESOIL, (4) two or three groundwater models, (5) two or three air models, and (6) an air-to-surface model has been proposed (Bonazountas 1981).

Two issues are worth consideration: (1) the temporal and (2) the spatial resolution of both the single medium models employed by a multimedia package and the multimedia package per se (Bonazountas 1981). These two issues frequently limit the general applicability of multimedia model, in a sense that so many input data are required that no user is willing to be subjected to this laborious and costly exercise.

Finally, when dealing with the notion of designing or (applying) a multimedia model, a developer is confronted with the optimal selection of single medium models, given: (1) study objectives, (2) data availability (3) modeling expenses, time, computational costs (4) mathematical constraints of single medium models employed, (5) expandable logic and model capabilities of the multimedia package, (6) calibration requirements of the multimedia package, and (7) clarity for model users.

4.4.6 Other Modeling Issues

Each of the compartment models discussed above deals with chemical properties and transformation coefficients. Transformation coefficients/rates and other parameters may not be available in the literature; therefore, model users may decide to compile these properties from a wide range of default values arranged by chemical class, and allow for a sensitivity analysis to provide decision makers with the relative importance of the process simulated in cases where no site specific input information exist.

Another issue is the input of materials balance data. The materials balance can be defined as an array of the release rates of chemicals from the industrial environment to the first point of entry into the natural environment, with geographical and temporal distributions specified. Two major components are encompassed by the materials balance; namely, the source identifications and the estimates of the environmental loadings. Factors such as geographic scale, industrial sector, environmental media, chemical class and time scale for release rate all combine to determine the scope and focus of a materials balance. In developing a materials balance approach, it is fundamental that all major sources--natural and anthropogenic, deliberate and fugitive--that can lead to potential exposure of sensitive geographic specific receptors be identified. Going beyond the identification, the release rate of these sources must be characterized in coordination with the "source/emissions" group of this study.

4.5 EVALUATION OF MONITORING DATA

Monitoring data provide information on toxics that is useful in all phases of a geographic toxics study, and the evaluation of monitoring data is an essential part of such a study. Without a monitoring data base, the problem identification and pollutant selection in the initial scan are more difficult. A good monitoring data base is necessary to validate and guide the sources and emissions inventory, the environmental pathways analysis, the exposure assessment, and the control strategies development. Furthermore, a toxics study supported by solid monitoring data is more likely to withstand legal and scientific scrutiny than a study without such data.

The evaluation of monitoring data should begin as soon as possible after the initiation of a geographic study, because this analysis will provide guidance and "feedback" to all subsequent phases of the study. A systematic approach that fully exploits the information available from the monitoring data is given below (with the exception of its use in the preliminary procedures, which is discussed in Section 2). The major steps in evaluating monitoring data are the same as for the sources and emissions inventory.

4.5.1 Definition of Needs

In the initial scan an effort to acquire all available monitoring data will have been made. Based on the current understanding of the potential toxics problems, decide which environmental pathways, exposure routes, and media are likely to be important with respect to the toxics problems in the area. The monitoring data needs should be prioritized based on these considerations. Ideally, a good monitoring data base is desirable for all potential exposure routes and environmental media, including ambient air, surface water, groundwater, soils and sediments, biota, drinking water, and food. In practice, however, resource and time constraints will limit the collection of new monitoring data and the investigator must decide which data bases are most important in a particular geographic area. For instance, if all the known toxics sources discharge exclusively to surface water, monitoring data on toxics in surface water, sediments, aquatic biota, and drinking water (if it comes from the polluted surface water) may be all that is necessary.

The minimum monitoring data base necessary for each selected media must also be determined. This will vary according to the nature of the toxics problem, and there are no fixed guidelines applicable to all studies. The following questions should be considered:

- Will the media be modeled? If so, what is the minimum number of sample locations necessary to adequately calibrate/validate the model? Are there certain geographic locations where monitoring data are needed?
- If the media will not be modeled but exposure will be assessed, what is the minimum number of sample locations needed to adequately characterize the environmental distribution and the degree of exposure? Are there specific sites where monitoring data are needed?
- What is the minimum number of samples and period of record needed to adequately characterize the average concentration and the range of concentrations for a particular sample site?
- What is the oldest acceptable age of monitoring data?

4.5.2 Review and Compilation of Data

After the minimum monitoring data needs have been established, all available monitoring data are compiled, media by media. As a first step, the number of samples, range of concentrations, and mean and median concentrations (if applicable) are compiled for each source/sample site. In the case of air and water, it may be useful to plot sources/sample sites on a map of the study area and note the geographic distribution of toxics concentration. This may elucidate trends (i.e., increase or decrease in concentrations in the downstream portion of a river) and indicate toxics 'hot spots'.

At this stage, reconsider the previously defined toxics problem in light of the monitoring data. Where possible, compare measured concentrations with existing environmental and health criteria. If the monitoring data base is comprehensive there may be adequate evidence to modify the source/discharge modes, environmental pathways, or exposure routes considered in the study.

4.5.3 Evaluate Adequacy of the Data

Once assembled, evaluate the monitoring data for each media with respect to the minimum data requirements established according to Section 4.4.1. If the minimum requirements are met, the data can be synthesized and interpreted as outlined in Section 4.4.5. Otherwise, plans must be made to acquire new data, as outlined below.

4.5.4 Design and Implement Plans for New Data Collection

If the minimum data requirements are not met, either revise the goals or plan to acquire new data. If new data are needed, design a sampling program that fills gaps while meeting the monetary and time constraints of the study. Coordinate sampling of ambient media to sampling of sources to provide the temporal and spatial relationships that support the establishment of a causal link. Developing a methodology for such a sampling program is beyond the scope of this study; it is recommended that EPA develop such a methodology, tailoring existing guidelines on sampling design to the geographic approach. The use of surrogate (regional or national) data is not recommended as a substitute for site-specific monitoring data, unless it can be conclusively shown that the surrogate data are representaive of local conditions.

4.5.5 Synthesize and Interpret Data

Once the complete monitoring data base has been assembled, evaluated, and expanded (if necessary), the synthesis and interpretation begins. This is a very important step because the monitoring data are the best tools for evaluating the accuracy of the source and emissions inventory, the environmental pathways analysis, and the exposure assessment. The actual procedure followed in the data synthesis and interpretation depends on the monitoring data base and the extent of modeling.

If a given media was not modeled, use the monitoring data to check on the sources and emissions inventory by: 1) qualitative comparisons and 2) performing rough mass balance calculations based on the source and emissions inventory and comparing these estimates with measured data. For the qualitative evaluation, compare ambient concentrations with the known sources of toxics to see whether emissions are reflected in ambient concentrations and whether any toxics detected through monitoring are not accounted for by the emissions inventory. The use of mass balance could be used for an unmodeled river, for example, by estimating toxics loadings from various sources in conjunction with known stream flow to develop a rough (order of magnitude) estimate of expected toxics concentrations, which can be compared to monitoring data. In the absence of modeling, use monitoring data to develop exposure levels and to assist in the development of control strategies.

For media that are modeled in the environmental pathway analysis, use the monitoring data to verify the emissions inventory, the modeling, and the exposure assessment. To verify the emissions inventory for a given media, find the location of the receptor/model compartment closest geographically to each monitoring site. Compile the predicted and measured concentrations for each pair of corresponding modeling/monitoring sites. Compare these predicted and measured values for the entire study area. If there are significant discrepancies between these data for one or more sites that may be due to incorrect emissions estimates, use the model as an investigative tool to site hypothetical undocumented sources of toxics or generate emission rates from known sources that more closely account for observed concentrations. Using this information try to find these sources, which were missed in the initial data gathering effort. Alternatively, if the resources of the study do not permit a computerized investigation with the model, perform a qualitative 'sensitivity analysis', by carefully examining the trends in modeled versus monitored toxic levels. Such an evaluation may suggest the possible reasons for the observed discrepancies.

If the comparison of modeling results with monitoring data suggests that there are significant discrepancies between the two that are due to problems in the modeling, use the monitoring data to calibrate or validate the model, if resources permit. It should be emphasized, however, that model calibration and validation can be expensive and that they generally require a very sound monitoring data base in order to be accurate. For example, the use of ambient monitoring data to enhance the predictive capability of atmospheric dispersion models is justifiable only if the monitoring data base is long-term (including at least one year of data), intensive (based on hourly sampling), and based on numerous well-located monitoring stations. In addition, comprehensive meteorological data must be available. In model calibration an attempt is made to adjust model estimates to better correspond with measured data. In this approach the reason for discrepancies between modeled and monitored data is not necessarily determined. A correction factor is developed using statistical methods (e.g., regression analysis) and implemented to improve the agreement with the monitoring data. Model validation, on the other hand, uses statistical tools such as time series analysis and correlation analysis to determine the reason for the discrepancy between modeled and monitored data and to adjust the model accordingly. The implementation of a validation includes the following steps: 1) comparison of measured and predicted values using a statistical package and a regression analysis; 2) determination of the cause(s) of any discrepancy involving emission data, meteorological data, or model; 3) correction(s) to the appropriate component; 4) rerun.

Finally, monitoring data can be used alone or in conjunction with modeling to pinpoint the problems that deserve consideration in the development of control strategies. This is discussed in Section 7.2.1.

4.5.6 Model Validation

Once the input data are complete, the models are run and the results have to be analyzed. Various methods are available for these analyses ranging from simple readings of output listings to sophisticated computer analyses of output on computer storage devices (tape, disk, data bases, etc.). The two major steps for analyzing/evaluating model outputs are model validation and model sensitivity analysis. The latter step is discussed in the next section.

Final model predictions should be validated for consistency with any available monitoring data (see Section 4.5). However, a disagreement in absolute levels does not necessarily indicate that either method is incorrect, or that either data set needs revision. Field sampling approaches and modeling approaches rely on two different perspectives of the same situation. Field data give a concentration at one point in time and space, models predict "average" concentrations for some particular conditions. Thus, field and model results may differ and still both be correct. Some possible reasons for a discrepancy are:

- The field sample was taken from a spot with atypical concentrations (e.g., a water sample may be 1.5 feet from a source, and so give abnormally high readings).

- The sample was taken under atypical conditions (e.g., on the one day/month that it rained); model results were calculated for average conditions, which rarely occur (e.g., coastal water studied at a mean tide level).

- The sample contained more than one phase (e.g., a water sample contained some suspended sediment).

The extraction procedure for the sample was under or over-efficient (e.g., it not only extracted all organic pollutants from a soil sample but also dissolved the soil).

Both types of data are important and convey different types of information. These data can be compared if the differing approaches are kept in mind.

4.5.7 Sensitivity Analysis and Scenarios

It is frequently worthwhile to perform sensitivity analyses to determine the effect on the predicted concentrations caused by a change in the input parameters. These sensitivity analyses are particularly important when data gaps or uncertain input values exist. It may also be useful to re-run the models to estimate the impact of various control strategies on toxics distribution and concentrations in the environment. Two main techniques are widely used to perform sensitivity analyses: (1) model simulations; (2) analytic techniques.

Model simulations are performed by running and rerunning the model, simultaneously varying the value of one or more parameters following a "scenario" logic. A typical scenario for a water compartment simulation is shown in Table 4-11. Model concentration predictions may be compared to monitoring data as described in the previous section.

Analytic techniques of linear systems theory (USDA 1973) and optimization theory (Haimes 1977) may correlate sensitivity of model input (e.g., effluent quantity) to model output (e.g., ambient concentrations) without performing multiple model reruns (simulations). An example of such a methodology is presented in Chapter 7 (Development of Control Strategies) of this report.

Table 4-11

A TYPICAL WATER SCENARIO

Water Scenarios: STREAMS REGION: ______________

PHYSICAL PARAMETERS	STREAM SIZES			
	Large	Med-Large	Medium	Small
Width, Meters				
Average Discharge - Q, Cubic Meters/Second				
Average Velocity, m/s				
Average Depth, m				
Low Q				
Low Velocity				
Low Depth				

CHEMICAL PARAMETERS in mg/l, Annual Data	Mean X	20% Value	80% Value	OBSERVED Minima	OBSERVED Maxima
pH					
Suspended Sediments					
Dissolved Solids					
Chloride					
Total $CaCO_3$ hardness					

SEASONAL DATA

Dissolved Oxygen:

February
April
August
November

Total Organic Carbon:

February
April
August
November

4.5.8 Monitoring Data Acquisition (Data Bases)

Monitoring data can be obtained from: (1) site specific sampling programs or (2) computerized data bases. Table 4-12 lists selected data requirements for a geographic pathway analysis, while Table 4-13 lists widely used computerized data (direct, indirect) bases. Direct data can identify areas where toxic pollutants have been found in the environment and at what concentrations. Indirect data can be used to identify areas where one might suspect that toxic pollution is occurring, i.e., by locating concentrations of industries which are suspected of contributing to toxic pollution.

Table 4-12

SELECTED DATA REQUIREMENTS OF PATHWAY ANALYSES

Class of Data	Possible Sources of Data
Pollutant Sources • Industrial surveys of manufacturers and users. • RCRA inspection forms. • Registration data. • Air quality emissions inventories.	Reports: TSCA inventory, SRI chemical directory, Radian report on Organic Chemical Producers, NEIC Kanawha Valley Study, NEIC follow-up report on 5 industries. Other: State offices, production and use reports, risk assessments, other materials balance from Chamber of Commerce.
Quantification of Emissions • Air: stationary source emissions permits, data from inspection/maintenance programs for non-point sources, compliance data. • Water: NPDES permits, other permits (state and local. Effluent Guidelines Documents. • Land: licensing or permit information for transport and disposal of hazardous and solid wastes. • Other: information on spills, pesticide accidents. Inspection reports.	Regional (EPA): Air Quality Monitoring Branch, Water Quality Monitoring Branch, Hazardous Waste Task Force, Enforcement Branches, Environmental Emergency Branch (Survey and Analysis Division), Pesticides Branch. [Also U.S. EPA Water Quality Analysis Branch for NURP and POTW Studies and Effluent Guidelines Division.] Also (USCOE) U.S. Corp of Engineers. State: Water Development Authority, Natural Resources Department (Water Resources, Air Pollution Control Commission. Others: Ohio River Sanitary Commission (ORSANCO), TSCA substantial risk notices, USGS Water Quality Alert, county and city offices, local planning agencies, contact with industries, other literature, county health offices, Bureau of Mines.

Table 4-12 (Continued)

Class of Data	Possible Sources of Data
<u>Environmental Fate</u> • Climatic data: i.e., precipitation, wind, wind speed, temperature, pressure, etc. • Hydrologic data: i.e., surface and ground-water distribution, quantity, etc. • Soil data: i.e., soil classification, geology, soil permeability, etc. • Land use data. • Chemical fate data: physical, chemical and biological properties of pollutants. • Monitoring data: concentrations of pollutants in environmental compartments.	<u>Federal</u>*: National Weather Bureau, NOAA, USGS, USDA (Soil Conservation Service), U.S. EPA Water Quality Analysis Branch (STORET/TOXET data bases, REACH, stream gages data), Bureau of Mines, USCOE. <u>State</u>: Natural Resources (Environmental Analysis, Water Resources, Wildlife Resources, Parks and Recreation), Geological and Economic Survey, Department of Agriculture (Soil Conservation Department, Air Pollution Control Commission, Water Development Authority. <u>Other Organizations</u>: University of W. Virginia, Ohio River Sanitary Commission (ORSANCO), county and city offices, literature (i.e., Versar fate documents, past risk assessments, other).

Table 4-13

DATA BASES OVERVIEW; PATHWAY ANALYSES

(1) DIRECT DATA

- AMBIENT MONITORING DATA

  Water

  - STORET - Storage and Retrieval of Water Related Data
  - NASQAN - National Stream Quality Accounting Network
  - Surface water monitoring
  - Monitoring to detect previously unrecognized pollutants in surface waters

  Air

  - SAROAD - Storage and Retrieval of Aerometric Data

  Soil

  - Ecological Monitoring System

  Groundwater

  - UIC/HWIS - Underground Injection Control/ Hazardous Waste Management Information System

- SOURCE SPECIFIC DATA

  Effluent Monitoring Data (water

  - Needs survey
  - IFB organic data base
  - Energy and mining point source category data base

  Emissions Monitoring Data (air)

  - NEDS - National Emissions Data System
  - HATREMS - Hazardous and Trace Emissions System

(2) INDIRECT DATA

- INDUSTRY BASED DATA

  - Data Collection Portfolio for Industrial Waste Discharges
  - EADS - Environmental Assessment Data Systems

4.6 SUMMARY AND CONCLUSIONS

The major steps in performing an environmental pathway analysis are:

(1) Collection of monitoring and site data

(2) Defining the important pathways in the Region

(3) Choosing models to simulate these pathways

(4) Compiling data to drive the models

(5) Analyzing the results

The results from this analysis can then be used as input to the Exposure Assessment Analysis (see Chapter 6), which evaluates the degree of human and other biotic exposure to toxic substances in a region, and as a basis for decisions regarding the environmental quality of the region. Therefore, an increased degree of collaboration is required between team members of the pathway analysis group and team members of both the pollutant source inventory and the exposure assessment groups, in order to select, discretize and apply models optimally.

Engineering judgment and professional experience are key factors for a successful pathway simulation. Given the current number of multimedia models it is advisable to perform multimedia simulation by appropriately selecting and interfacing single medium models rather than seeking immediate use of an existing multimedia package that can be very costly (professional time, computer cost) and may not be directly applicable to a study.

Study duration is a function of: (1) the study area (size, complexity, location), (2) data availability , and (3) professional experience of performing organization (agency, consultant). A period of 3 to 5 months appears to be a reasonable estimate.

A pathway analysis requires an interdisciplinary team of:

(1) a senior task manager specializing in modeling of at least two environmental compartments (e.g., soil and water), who will be also effectively involved (as a subtask leader) in one of them;

(2) three subtask leaders (project manager in one) for the air, soil/groundwater and water compartments;

(3) three junior scientists for data compilation (environmental scientist) computer programming, model runs (computer scientist) and output analysis (environmental scientist); and

(4) secretarial and support staff

Large memory computer systems, computer graphic facilities, and word processors are valuable tools for a cost effective performance, since models would probably have to be run multiple times in light of errors or new information discovered in input data. Therefore, graphs would have to be reproduced and reports retyped in light of corrected output.

4.7 REFERENCES

Aravamudan, K., M. Bonazountas, A. Eschroeder, D. Gilbert, L. Nelken, K. Scow, R. Thomas, W. Tucker, C. Unger (1980); "An Environmental Partitioning Model for Risk Assessment of Chemicals," Arthur D. Little, Inc., Cambridge, MA 02140 under EPA Contract 60-01-3857 for Office of Toxic Substances, Washington, DC 20460.

Bonazountas, M. (1981); "A Multi-media Environmental Modeling Background/ Catalogue," Internal Document, Arthur D. Little, Inc., Cambridge, MA 02140.

EPA/MIBS (1981); "Environmental Modeling Catalogue," EPA, Management Information and Data Systems Division, Washington, DC 20460.

EPA (1980); "Handbook for Performing Exposure Assessment," the EPA's Exposure Group; An unpublished document.

Haimes, Y.Y. (1977); "Hierarchical Analyses of Water Resources System," McGraw-Hill Series in Water Resources and Environmental Engineering, McGraw-Hill, New York.

Miller, C. (1978); "Exposure Assessment Modeling, A State-of-the Art Review," EPA, Athens Research Laboratory, EPA PB 600/3-78-065.

USDA (1973); "Linear Theory of Hydrologic System," Technical Bulletin No. 1463 (Stock #0100-02747), USDA, Washington, D.C.

5.0 RECEPTOR/EXPOSURE ROUTE ANALYSIS

5.1 INTRODUCTION

The purpose of the Receptor/Exposure Route Analysis is to define critical exposure pathways for toxics in a specified region and describe methods for estimating exposure through these routes, for both human and nonhuman receptors. The results of this task combined with the output from Task 3 serve as the primary input to Task 5, the Exposure Assessment. The data prepared in this task are not, for the most part, pollutant-specific but, in some cases -- such as the population characterization -- are necessarily regionally specific.

The two discrete subtasks within Task 4 are: 1) selection of algorithms for estimating individual intake levels of pollutants for each exposure pathway; 2) determination of the regional distribution of study area receptor populations, and characterization of the temporal, behavioral and other patterns influencing their exposure through each pathway.

Exposure assessment methodologies and handbooks have been developed for various government agencies and private organizations and, although most are not regional in scale, they are useful resources in developing any exposure assessment approach. Relevant sources are listed in Table 5-1. The purpose of this section is not to reiterate the general exposure assessment methodologies compiled in prior studies, but to develop a region-specific approach and to relate it to existing methods wherever appropriate.

There are several immediately apparent differences between a geographically-based exposure assessment methodology and other methodologies intended to estimate national or generic exposure to a specific chemical, industry, commodity, or other categories. A geographic assessment is conducted on a small enough scale to develop detailed and accurate receptor population data regarding the size of exposed populations and the spatial relationships of receptors to points of pollutant release.

TABLE 5-1

REVIEWS OF HUMAN EXPOSURE ASSESSMENT METHODOLOGIES

Title	Source
Guidance for the Preparation of Exposure Assessments	EPA Exposure Assessment Group (1980)
Handbook for Performing Exposure Assessments (Preliminary Draft)	EPA Exposure Assessment Group (1980)
Report on Exposure Assessment Status and Principles[1]	Consumer Product Safety Commission (CPSC) (1981)
Proceedings of Workshop on Exposure Assessment of Hazardous Chemicals[2]	U.S. EPA (1980)
Integrated Exposure/Risk Assessment Methodology (Preliminary Draft)	Monitoring and Data Support Division, Office of Water Regulations and Planning, EPA (1980)

[1] Cited in EPA (1980).

[2] By Radian Corporation (1980), EPA contract No. 68-02-3171.

Also, generalized expressions of annual pollutant intake rates can be "calibrated" for the study area by adjusting for regional patterns of recreation, food-consumption, occupation, transportation and other activities. These region-specific intake rates enable a more accurate estimate of local exposure than generalized average intakes.

5.2 EXPOSURE ROUTES AND EXPOSURE MEDIA

5.2.1. Introduction

Following the initial scan and data retrieval effort (described in Section 2.5), a set of critical exposure routes and receptors will have been identified for the geographic area being studied. For each combination of an exposure route and a specified environmental medium (e.g., ingestion in drinking water), the general equation for estimation of the individual pollutant intake via this pathway will be:

$$I_P = I_{EX} \cdot P_{EX}$$

where: I_P = pollutant intake rate

I_{EX} = exposure medium intake rate

P_{EX} = pollutant concentration in exposure medium

The exposure medium intake rate may be expressed simply as a unit mass per day (e.g. for ingestion), or with more detailed information, as:

$$I_{EX} = I_{EX^1} \cdot F_{EX} \cdot D_{EX} \cdot E_{EX} \cdot A_{P,EX}$$

where: I_{EX^1} = unit exposure medium intake rate per exposure event

F_{EX} = frequency of exposure events (number of events/time)

D_{EX} = duration of exposure event (time)

E_{EX} = extent of exposure (%)

$A_{P,EX}$ = efficiency of absorption of pollutant for that exposure route (%)

The second equation is more applicable to exposure through dermal absorption than through other exposure routes. The reasons are discussed in Section 5.2.2.4.

The time period to use in estimating and grouping pollutant intake values is determined by the eventual application of the exposure results. Exposure medium intake rates may vary on a daily (e.g. for inhalation) or seasonal (e.g. for recreational dermal absorption) basis. If the variability has a significant influence on pollutant intake rates, then exposure should be calculated in small enough time-steps to reflect these differences.

The absorption efficiency term allows estimation of the effective dose or the amount of pollutant which crosses the membrane of the exposed tissue (e.g. the lung) and reaches a target organ (e.g. the liver). For many pollutants this type of metabolic data is not available and consequently 100% absorption is a common preliminary assumption in exposure assessments. For well-studied substances such as radionuclides, a methodology for calculation of exposure levels has been developed for specific organs including bone marrow, lungs, endosteal cells, stomach wall, lower intestine wall, thyroid, liver, kidney, testes and ovaries as well as for the total body (Moore et al. 1979). If individual absorption coefficients have been measured for the transfer of a pollutant into the lung or stomach or across the dermis, these factors can be included as efficiency coefficients in the calculation of doses rather than simply intake levels.

Intake can be expressed either as a pollutant mass per unit time, as discussed above, or as a mass per kg of body weight per unit time. The latter expression facilitates comparison to health effects data, especially laboratory animal data, which are commonly reported in equivalent units. Similarly, depending on the route of exposure, intake may be estimated on an annual basis to address chronic effects, or on a smaller time scale for addressing acute effects inclucing lethality, teratogenesis, reproductive and neurotoxic effects.

It may not always be desirable to express exposure as a pollutant intake level. For some types of exposures and receptors, such as fish, health effects data are commonly available in the form of concentrations in the exposure media, for example as an LC_{50} (a pollutant level in water lethal to 50% of the experimental population). The relationship between toxicity and the amount of pollutant absorbed by the gill in a unit period of time is rarely determined. Similarly, the relationship between pollutant levels in food and adverse effects on fish is not well understood. Therefore in the case of aquatic species, it is appropriate to report exposure levels as a concentration in water for easy comparison to effects data.

The magnitude of exposure in a geographic area is a function not only of the amount of pollutant to which an individual is exposed but also of the size of the population exposed. Therefore, it may be useful to express exposure on a population basis, thus accounting for the number of receptors exposed to a particular pollutant level. The resulting quantity is a <u>population exposure factor</u> which is the product of the individual pollutant intake level per unit time multiplied by the population size exposed. Exposure factors enable comparison of the magnitude of exposure in different regions or for various subpopulation categories and, consequently, helps identify the most significant local exposures.

The following subsections describe the methods commonly used to estimate intakes for each exposure route, and some of the input parameters required to make the calculations. Also potential sources for input data are identified. Each major exposure route is treated individually.

5.2.2 Humans

5.2.2.1 Introduction

The methods used to calculate exposure levels for humans are relatively independent of the type of exposure assessment (e.g., regional vs. national) requiring these data. Therefore, the methodologies and models developed for other exposure applications are relevant to a regional exposure assessment. Existing models are briefly discussed by exposure route in the following section. The EPA Exposure Assessment Group has compiled an initial draft of a Handbook for Conducting Exposure Assessments which contains parameters and expressions for estimating intakes currently being used in EPA work. A second draft will be published in the near future. This document along with other references listed in Table 5-2 and 5-3 provide more detailed documentation of relevant methods and parameters, along with examples of their application to different types of exposure assessments.

5.2.2.2 Ingestion

A common exposure route through which humans are exposed to pollutants is ingestion of contaminated drinking water or food. Other less typical ingestion-related exposures can occur through mouthing of soil (e.g. by children), swallowing of saliva during exposure to high airborne concentrations of pollutants, swallowing of water during tooth-brushing or participation in water-contact sports. Only drinking water and food are discussed in this section.

In a regional exposure assessment, drinking water supplies and certain area-grown foods are examples of potentially important exposure media which can be related to the local sources and emissions of toxics. Questions may arise regarding the effectiveness of drinking water treatment methods employed to prevent contamination of water supply, or regarding the contribution of local foods to the total diet intake of a specific pollutant. The environmental pathways leading to contamination of these media are often complex and indirect, involving a series of intermedia transfers. An example is the transfer of pollutants from a land disposal site into a ground water aquifer used as a water supply. Without the implementation of a fate model, it may be difficult to relate toxics concentrations back to a specific source.

TABLE 5-2

SPECIFIC HUMAN EXPOSURE ASSESSMENT METHODOLOGIES

TITLE	OFFICE	EXPOSURE ROUTES AND PATHWAYS CONSIDERED
Methodology for Estimating Direct Exposure to New Chemical Substances	Office of Toxic Substances, EPA (III); EPA 560/13-79-008	Inhalation, ingestion and dermal absorption for occupational and consumer populations
AIDOS-EPA: A computerized Methodology for Estimating Environmental Concentrations and Dose to Man from Airborne Releases of Radionucleides	Office of Radiation Programs, EPA; EPA 520/1-79-009	Inhalation, ingestion of foods and drinking water, dermal absorption. Transport from environment to food was modelled.
CUMEX-A Cumulative Hazard Index for Assessing Limiting Exposures to Environmental Pollutants	Environmental Sciences Division, Oak Ridge National Laboratory, ORNL Publication No. 1007	
Technical Support of Standards for High-Level Radioactive Waste Management Volume C, Migration Pathways	Office of Radiation Programs, EPA; EPA 520/4-79-007C	Ingestion of water and food. Transport from environment to food and water was modelled.
Human Exposure to Atmospheric Concentrations of Selected Chemicals	Office of Air Quality Planning and Standards, EPA	Inhalation
Environmental Carcinogens and Human Cancer	Office of Research and Development, Health Effects Research Laboratory, PB-291-742	Inhalation
Mathematical Models for Atmospheric Pollutants	Electric Power Research Institute (EPRI), Palo Alto, California	Inhalation, exposure of biota to airborne pollutants

TABLE 5-3

SOURCES OF DATA ON HUMAN INTAKE RATES AND PARAMETERS

FASEB 1972. Biology Data Book. Volume III.

FDA. Total Diet Studies. Compliance Program Evaluation. Bureau of Foods, Washington, D.C.

National Center for Health Statistics (NCHS). 1977. Dietary intake findings. Data from the National Health Survey. Series 11, number 202.

National Center for Health Statistics (NCHS). 1979. Dietary intake source data. Findings of the Health and Nutrition Examination Survey (HANES). DHEW publication no. (PHS) 79-1221.

Roddin, M.F., H.T. Eclis, N.W. Siddizee, and R. Lieberman. 1979. Background data for human patterns. Prepared by Stanford Research Institute under Contract No. 68-02-2835. U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, N.C.

Task Group of Committee 2 of the International Commission on Radiological Protection. 1975. Report of the Task Group on Reference Man. Pergamon Press: New York.

USDA. 1972, 1980. Food and Nutrient Intakes of Individuals in the United States. Agricultural Research Service, Washington, D.C.

U.S. EPA. 1979. Identification and Evaluation of Waterborne Routes of Exposure from other than food and drinking water. Office of Water Planning and Standards, U.S. EPA, Washington, D.C.

Yost, K.J. and L.J. Miles. 1980. Dietary consumption distributions of selected food groups for the U.S. population. Prepared by Purdue University under Contract No. 58-01-4709. U.S. Environmental Protection Agency, Office of Toxic Substances.

TABLE 5-4

COMMONLY USED INTAKE RATES

FOR INGESTION OF SELECTED

EXPOSURE MEDIA

Exposure Medium	Typical Intake Rates	Individual Variability	Probable Seasonal Variability
Drinking Water[1] (total fluids)	Average: 2 l/day	Adult Range: 1.1 - 2.4 l/day Children: 1.1 - 1.7 l/day Moderately active individual: 3.7 l/day Under high temperatures: 2.8 - 3.4 l/day	Annual average exposure; higher rate during summer (+50%)
Meat, Poultry and Fish[2]	Average: 200 gm/day	Adult range: 310 g/day Children: 70g - 150 g/day	Annual average exposure; probable higher intake of local fish during summer.
• Beef	Average: 54 g/day		
• Pork	Average: 20 g/day		
• Lamb, veal, game	Average: 2 g/day		
• Poultry	Average: 27 g/day		
• Fish, shellfish[3]	Average: 11 g/day		
• Others	Average: 94 g/day		
Milk and Milk Products[2]	Average: 270 g/day	Adult Range: 250g - 650 g/day Children: 400-800 g/day	Not significant
Eggs[2]	Average: 27 g/day	Adult Range: 15g - 55g/day Children: 5g - 22g/day	Not significant
Legumes, Nuts and Seeds[2]	Average: 26 g/day	Adult range: 5-45g/day Children: 20g - 65g/day	Not significant
Grain products[2]	Average: 200 g/day	Adult Range: 150g - 250g/day Children: 40g - 200g/day	Not significant
Fats, oils[2]	Average: 14 g/day	Adult range: 10g - 19g/day Children: 1g - 9g/day	Not significant
Vegetables[2]	Average: 200 g/day	Adult Range: 140 g - 285 g/day Children: 75g - 135 g/day	Annual average exposure; probable higher intake of locally grown produce during summer.
• White potatoes	Average: 64 g/day		
• tomatoes	Average: 22 g/day		
• dark green	Average: 9 g/day		
• deep yellow	Average: 6 g/day		
• others	Average: 99 g/day		
Beverages[2,4]	Average: 600 g/day	Adult Range: 300g - 840 g/day Children: 50g - 270 g/day	Annual average exposure; probable higher intake during summer
Fruits[2]	Average 140 g/day	Adult range: 105-190 g/day Children: 135g - 170 g/day	Unknown
Sugar, sweets[2]	Average: 23 g/day	Adult range: 14g - 42g/day Children: 10g - 27 g/day	Not significant

[1] Report of Task Group on Reference Man (1975)

[2] Average intake per individual in a day, Spring 1977 (USDA 1980)

[3] U.S. EPA recommends using 6.5 g/day

[4] Some portion of this intake will be included under drinking water (total fluids)

The rate of ingestion or intake of a specific exposure medium is a function of the particular medium or food group consumed. Table 5-4 summarizes commonly used intake rates for drinking water and selected food groups, the potential for variability by age, sex, or region in each rate, and the seasonality or temporal component of these rates.

Since food consumption patterns vary regionally, both in terms of the items and the amounts that people consume, a more localized approach than the one described above may be desired. An FDA one-day survey of U.S. consumption patterns by region, sex, age, income and season for a number of food items was conducted in 1965-66 (FDA 1973), and again in 1977 (data still preliminary; FDA 1980). These data make it possible to quantify the consumption rate of numerous food groups and the size of the population consuming each food group in four major U.S. regions.

Populations exposed to drinking water can be estimated from water supply distribution information, permits, and laboratory records from the state and local authorities and/or water supply companies. Populations exposed through ingestion of specific food groups can be estimated from generic data on consumption patterns for the general population, from regional data developed by the FDA study described above, as well as from contacts with local sources.

5.2.2.3 Inhalation

Intake of toxics may occur through inhalation of ambient air contaminated by emission plumes at locations downwind from specific industrial point sources. Exposure may also occur during the use of volatile or sprayed consumer products and in the vicinity of non-point applications or releases, e.g., downwind from pesticide treatments, dry cleaning operations, or heavy traffic. The general population may also be exposed to ambient "background" levels not directly associated with specific sources. Inhalation of mist, fog, and vapors in contaminated air associated with contaminated water bodies, drift from cooling towers, etc., may also contribute to pollutant intake.

In comparison to other exposure media, air is a relatively uniform, continuous medium to which all humans are exposed 24 hours per day. The amount of pollutant taken into the body is a direct function of the rate of inhalation volume of air inspired per unit time, which is in turn a function of the metabolic rate. Table 5-5 presents some rates commonly used in exposure assessments. Higher rates may occur at high temperatures or during strenuous exercise. Slightly lower rates may occur in people with respiratory diseases and in the elderly. Exposure assessments commonly employ either a single daily inhalation rate averaged over a 24-hour period or a daily rate combining a period of strenuous exercise (high rate) with a sedentary period (lower rate).

Residential population data by census division, such as the information collected in the census bureau surveys, is commonly used to estimate the size of receptor populations exposed to pollutants in a localized area. Adjustments can be made to the population estimates to account for receptor mobility over daily or longer time periods. A discussion of the use of demographic data in geographic exposure assessments follows in Section 5.4.

5.2.2.4 Dermal Absorption

Exposure to toxics through dermal absorption may occur during swimming or other water-contact sports in surface water, during washing and bathing in water supply, and during use of consumer products (liquids and vapors) or contact with items treated with such products. Intake of any substance through dermal absorption is a function of the extent, frequency and duration of exposure. The extent parameter (E) indicates the portion of the body (most commonly measured as percentage of total surface area) in contact with the exposure medium and hence the area at which absorption through the skin will occur. A common range for this variable is from 10% for hands to 100% for the total body surface (EPA 1979). For recreational activities such as swimming and water skiing, during which immersion is nearly total, E may be set at 100%.

TABLE 5-5

INHALATION RATES FOR HUMANS BY ACTIVITY AND SEX[1]

	ADULT MALE	ADULT FEMALE
Body weight (kg)	68.5	54.0
Experimental conditions	light work medium work heavy work	light work medium work heavy work
Respiratory frequency (breaths/min)	11.7 (10.1 - 13.1) 17.1 (15.7 - 18.2) 21.2 (18.6 - 23.3)	11.7 (10.4 - 13.0) 19 30.0 (25.0 - 35.3)
Tidal volume	750 (575 - 895) 1673 (1510 - 1770) 2030 (1900 - 2110)	339 (285 - 393) 860 (836 - 885) 880 (490 - 1270)
Minute volume (liters/min)	7.43 (5.8 - 10.3) 28.6 (27.3 - 30.9) 42.9 (39.3 - 45.2)	4.5 (4.0 - 5.1) 16.3 (15.9 - 16.8) 24.5 (17.3 - 31.8)

[1] Source: FASEB's Biology Data Book, Volume III, 1972

Frequency (F) and duration (D) give the total amount of time each year during which exposure of an individual is occuring. Frequency is the number of events in a unit time period an exposure activity takes place, and duration is the time period (usually hours) for each activity. The product of these terms gives hours of individual exposure per year.

For dermal absorption, either one of two methods is used for estimating the pollutant intake. The more reliable method incorporates a measured permeability rate constant for dermal absorption of the particular pollutant -- expressed in units of $\mu g/cm^2/hr$ -- into the equation, assuming low pollutant concentrations and an equivalent dermal absorption across all areas of skin (U.S. EPA 1979). These measurements are usually made in vitro with intact skin and may not accurately represent in vivo behavior.

The second, less precise, method for estimating dermal exposure is to assume pollutant diffusion across the skin at a rate equal to the rate of diffusion for the solvent, in this case water, which equals 0.2 to 0.5 $mg/cm^2/hr$ (U.S. EPA 1979). This method may underestimate the exposure of some substances, especially those that are highly lipophilic or have a high octanol/water partition coefficient.

The identification of the population exposed via dermal absorption does not usually involve geographic subdivisions, as in the case of sub-populations exposed to air. Receptors are individuals who through their behavior or activity patterns, rather than as a function of where they live, come into temporary dermal contact with exposure media during specific activities such as recreation, use of products, bathing, and others. Survey data on the recreational use of beaches, use of home pesticides, etc., and information on the population served by a water supply would be the type of information required to quantify these groups.

Pollutant concentration data measured in water and in consumer products are available from several sources. Monitoring data for water supplies are usually available from the state and county drinking water offices. Surface water data can be found in the STORET water quality data base, at the EPA regional office, at state environmental departments and sometimes from private organizations. Information on pollutant concentrations or exposure levels associated with the household use of selected pesticides has been developed by the Special Pesticides Program, Office of Pesticide Programs, in conjunction with their RPAR[1] program. The methodologies developed to estimate exposure are applicable to other substances as well.

5.2.3 Other Biota

In a regional exposure assessment it may be important to identify the exposure and risk of fish, wildlife, plants and other nonhuman species to toxic pollutants for several reasons. Certain sensitive species may provide an early warning signal for a local toxics problem, as indicated by mortality or accumulated toxics levels in tissue. Protection of crops, sport fisheries, game, and livestock are of interest because of their economic value to man. Most importantly, environmental quality is a function of the diversity, abundance and productivity of indigenous species in a community, so the preservation of the existing ecosystem, or at least part of it, is desirable. In some cases, the exposure of abiotic receptors, such as buildings, works of art, or other inanimate objects may be of concern in a geographic exposure assessment.

Identification of critical nonhuman receptors is very region-specific and dependent on the species present and the number of individual habitats to consider. In general, far less extensive population surveys are conducted for nonhuman populations than for humans. Therefore, during the screening for species of concern in a specific geographic area, some of the factors which may be considered include presence in the area of endangered or threatened species, agricultural land use (either for crops or raising livestock), or presence of sensitive or critical

[1] Rebuttable Presumption Against Registration

habitats (e.g., wildfowl nesting or fish spawning area; resting/feeding areas along migration pathways). In industrial or highly populated areas, a potentially critical receptor category may be the microbial populations in POTWs and industrial secondary treatment processes.

Table 5-6 lists some of the species categories which may be considered in a geographic assessment and the critical exposure routes of concern for each group. Since there are numerous pathways in a specific area, many interrelated, which link a toxic from source to receptor, the focus may be limited to only critical routes. Critical routes are those either involving a large mass of pollutant or leading to exposure of sensitive or economically important receiptors, or of large numbers of receptors.

Ecosystem models have been developed for both generic ecosystems (e.g. freshwater lakes, prairies) and specific locations (e.g. the Upper Mississippi, Rocky Mountain Arsenal). Ecosystem models are useful for understanding the impact of exposure on an entire, integrated biotic system and to evaluate indirect impacts (such as reduction in an important food source, inhibition of nutrient cycling). Several major problems limit the use of such models, including nonlinearity, limited data for many of the processes, the spatial and temporal resolution of different processes, and lack of a general theoretical basis to support inclusion of some of the parameters influencing ecosystem dynamics. Physical system models are generally at a far more advanced state than biological models because they do not have many of the problems described above. An ecosystem model of the geographic area being studied would enable a detailed and organized assessment of the local impact of toxics. However, these models are only available for limited locations and are probable too expensive and time-consuming to develop within the course of geographic assessment.

TABLE 5-6

EXAMPLES OF NONHUMAN RECEPTORS TO BE CONSIDERED IN AN EXPOSURE ASSESSMENT

Receptor Group	Examples	Important Exposure Routes[1]	Exposure Media[1]
Aquatic Communities:			
• Fish and other vertebrates	Warm water species, salmonids, amphibians	<u>Absorption</u> (gill and dermal) ingestion	<u>Surface waters</u> (natural systems), impoundment water, sediment, other biota
• Invertebrates	Molluscs, crustaceans	<u>Absorption</u>, (mantle and dermal) and ingestion	<u>Surface water</u>, sediment, oth biota
• Producers and primary consumers	Algae, macrophytes, zooplankton	<u>Absorption</u>, ingestion	<u>Surface water</u>, sediment, oth biota
• Waterfowl and other birds	Ducks, geese, gulls, predators such as osprey, eagles	<u>Ingestion</u>, dermal absorption (oil)	Surface water, <u>fish</u>, <u>plants</u>, and other biota
Terrestrial Communities:			
• Crops	Leafy vegetables, root crops	<u>Cuticle absorption</u>, <u>root uptake</u>	<u>Soil</u>, <u>fallout</u>, rain, irrigation water, pesticides
• Indigenous plant communities	Wetlands, forests	<u>Cuticle absorption</u>, root uptake	<u>Soil</u>, fallout, rain, pestici
• Livestock	Dairy and beef cattle, chickens	<u>Ingestion</u>, dermal absorption, inhalation	Surface water, <u>water supply</u>, locally grown feed and fodde pastures, medicinal applications, pesticide-treated pro ducts
• Wildlife	Songbirds, hawks, deer	<u>Ingestion</u>, dermal absorption, inhalation	Surface water, <u>other biota</u>, pesticide drift
Microorganisms			
• Natural Communities	Bacteria (e.g., nitrifiers), fungi	<u>Absorption</u>	<u>Surface water</u>, sediment, <u>soi</u>
• Waste-water treatment populations	in POTWs	<u>Absorption</u>	<u>POTW influents</u>, <u>wastewater</u>

[1] The underlined items are those most commonly considered in exposure assessments

5.3 RECEPTOR POPULATION CHARACTERIZATION

5.3.1 Humans

5.3.1.1 General Population

An important part of a geographic assessment is the development of a detailed and up-to-date human demographic data base for the area being studied. These data can provide the basis for estimates of subpopulations associated with different exposure routes. In many exposure assessments it is common to use an average population density for the total U.S. or to simply distinguish between rural and urban densities. In a geographic exposure assessment in which site-specific data on pollutant releases, environmental fate and ambient levels are measured or estimated, it is important to have equally detailed population data.

Availability of data from the 1980 census permits detailed analysis of populations exposed to pollutants. By the early fall of 1981 population breakdowns by age, sex, and housing units should be available for use in an exposure analysis. The data are grouped into five major divisions for each state, county, tract, enumeration district/place, block group and block.

Census tracts tend to cover fairly large areas in each state, containing on average from 2,500 to 8,000 residents; tracts are used both to subdivide densely populated areas and to cover large rural areas which are sparsely populated. These larger rural tracts are further broken down into enumeration districts and places. Enumeration districts on average do not exceed a population of 1,000. Places are dense concentrations of population, primarily towns, which appear as distinct highly localized areas within a tract. The majority of medium-sized towns in a state are identified by place codes. Larger cities are also identified by a place code but are further disaggregated into a number of smaller tracts.

The lowest level of detail in very densely populated areas is provided by the block groups and blocks. In general blocks comprise an area bounded by four streets and are aggregated into block groups. To create special study areas for individual cases block groups and blocks can be subtracted from one tract and added into a population division that is entirely within an exposure assessment study area. Block groups can also be used to subdivide area tracts which are so large that they cannot be reasonably represented with a single exposure or concentration value.

In order to understand the exact location of each census division, detailed maps are provided by the Census Bureau which show exact boundary locations; these often include streets, train tracks, power lines, political boundaries and topographical features such as streams and rivers. When final versions of the data have been released, population centroids expressed in longitude and latitude will be provided to allow approximate boundary placement without maps. This will facilitate any computerized analysis of these data that is sensitive to locations.

A geographic region's population can be assumed to be static -- that is, not dependent on mortality, mobility or birth patterns -- for short-term exposure periods (e.g. <1 year). For the longer periods of exposure which are of interest in a chronic study (e.g. from approximately one year to a human life-span), time-dependence can be included in the demographic model. Therefore, variations can be accounted for in the total population size and distribution due to birth, death and migration processes as well as changes in the distribution of age, sex, racial, sociological and other classes. On a geographic scale, it is likely that detailed information is available from the Census Bureau and land use studies to estimate historical population fluctuations as well as to predict future trends. In addition, general mathematical models have been developed to estimate population dynamics, for example those described in Pielou (1969) and Pollard (1973). Population fluctuations over a shorter time period, such as changes with the movement of the working-age population, may also be important to include in a geographic study. Horie and Stern (1976) have published one approach to this problem.

5.3.1.2 Special Subpopulations

Within the general population of any given region, it may be important to quantify special subpopulations associated with specific types of exposure. Sources for data on these groups are summarized in Table 5-7. The subpopulations can be divided into at least two categories: sensitive groups and specific exposure-related groups.

The sensitive subpopulations are those that because of their age or health characteristics (e.g., very young or old age, poor health) have the potential to be at greater risk when exposed. These groups can be identified within a geographic region and, therefore associated with an exposure level for that area. School children can constitute up to 20% of a regional population and spend as much as 8 to 10 hours daily at the school grounds. School locations and associated attendance can be obtained from local, county or state boards of education. Elderly persons in nursing homes also represent an increasingly important segment of the population. Data on nursing home facilities are commonly maintained by State health service agencies and county or local boards of health, including geographic location and size of facility. In the absence of such summary data, the yellow pages of the telephone book are, at the least, a source of identification of nursing homes. Sensitive populations located at hospitals (general and specialized care) can be estimated through information from State health service agencies or boards of health, who can provide data on hospital locations and level of activity, including: number of beds, average length of stay, statistics on types of disorders, outpatient visits and emergency room activity.

Specific exposure-related subpopulations may be estimated from survey information on activity or use rates as well as from census bureau statistics. Recreational activity in a region occurs in state, county, or town/city parks and recreation centers and at privately maintained recreational facilities (tennis, golf, swimming, fishing, hunting clubs). Information on attendance (by month of the year) and location of recreational facilities can be obtained through many of the public agencies listed in Table 5-7 or from the private facility operators. Data on the use of specific products of significance in geographic exposure may be more difficult to obtain and require contact with the manufacturer or with local vendors of the product. Employment-related exposure populations may be estimated from data available through the U.S. Bureau of Census, County Business Patterns, and through state employment security divisions. Often, available information provides location of a firm or plant and associated employment. Because employment information at the local level is occasionally sensitive (due to business confidentiality) and unavailable, assumptions can be made using employment totals for a community and using land use maps to estimate geographical distribution patterns.

5.3.2 Other Biota

Population data for flora and fauna present in a geographic area provide a basis for assessing the impact of local pollutant concentrations within various subregions in terms of total numbers of individuals (e.g., fish) or acres (e.g., for crops) exposed and whether or not sensitive age classes, reproductive stages, species, or other groups are exposed. Receptors can be considered individually by species or as entire communities, depending on the eventual application of the exposure estimates, e.g., whether pollutant effects on a particular species or on the species diversity index for a particular habitat are of interest.

Table 5-6, presented earlier, listed examples of nonhuman receptors that may be of interest in a regional exposure assessment. Populations of these receptors within a region can be estimated from agricultural statistics, from USDA extension offices or local universities, and from contacts with local fisheries and wildlife resource offices,

TABLE 5-7

SOURCES OF DATA FOR CHARACTERIZING HUMAN RECEPTOR POPULATIONS

Receptor Category	Source of Data
General Population Regional Subpopulations	U.S. Census Bureau, Council of Governments; local planning agencies (county, community)
Sensitive Subpopulations	County and Community Boards of Education; State Department of Health Services; County Board of Health; Health department at local universities
Recreational Subpopulations	State, County, and Community Recreational Commissions; local Chamber of Commerce; State Department of Natural Resources
Occupational Subpopulations	State Division of Employment Security; State Manufacturing Directory
Subpopulations by Food and Water Consumption Patterns	USDA Nationwide Food Consumption Surveys; State Office of Drinking Water; county and community Drinking Water Divisions; water supply companies.
General Information	Phone books, local universities; local industries, recreational facilities and health care facilities.

U.S. Fish and Wildlife Service, National Park Service, U.S. Forest Service and other agencies. Information on crops and domesticated animals is usually better documented, more readily available and accurate than information on natural populations. For the latter, data consist primarily of results from mark and recapture or other sampling surveys, for small areas and limited time periods. Due to the variability in types of communities within a region, population data representative of all habitats may not be available, and rough estimates based on comparable biological communities in other areas may be employed.

6.0 EXPOSURE ASSESSMENT

6.1 INTRODUCTION

The Exposure Assessment is the fifth step in the analysis of regional exposure to toxics. In this step, the data and methods developed in the previous tasks are linked together in order that the relationship between local sources of toxics and the exposure of humans and other biota living in that locale can be examined. Through estimation of the degree of exposure rather than mere consideration of pollutant concentrations in environmental media, a more detailed analysis is possible including:

- evaluation of whether or not the toxic ends up in significant exposure media or at locations at which exposure takes place;
- estimation of the amount of toxic to which a receptor is exposed in a unit time period, including a cumulative total for chronic exposure;
- consideration of the influence of receptor behavior patterns or environmental conditions on receptor exposure.

The ultimate goal of evaluating a toxics problem in a particular area is to identify and evaluate potential adverse impacts on humans, fish and wildlife, plant communities and other species. Therefore, determining the nature and extent of toxics exposure is a logical first step toward assessing these impacts.

6.2 PURPOSE OF AN EXPOSURE ASSESSMENT

The overall purpose of the Exposure Assessment is to estimate the magnitude of exposure of receptors, both human beings and other biota, to toxic pollutants distributed throughout the environment of a specified region. This includes specific consideration of all potential exposure media such as air, drinking water, surface water, sediment, soil, plant and animal food products and consumer products as well as a combined or total exposure through all media, if possible.

Exposure is ideally estimated at all points of potential contact with receptors in the pathway leading from a chemical's points of release to its final equilibrium distribution in the environment. Figure 6-1 illustrates the environmental pathways of a pollutant and locations of potential exposure. The input concentration data required for these estimates can be actual monitoring concentrations and/or estimated levels predicted by environmental fate models. The advantage of monitoring data is that they give known levels found in exposure media; however their relationship to sources and the extent to which they are representative of regional levels are uncertain. Estimates from fate models have the advantage that their relationship to sources can be investigated through sensitivity analyses; however they are often difficult to validate.

For certain exposure pathways, the spatial distribution of differentially exposed receptors within the study area is of interest. This information is useful for populations exposed through inhalation or dermal absorption from surface water, two exposure pathways which usually have a spatial variability in their associated pollutant concentrations. If a number of water supplies (e.g., private wells) serve one study area population, the distribution of the associated receptors may also be important. On the other hand, exposure media that are channelled to a central location before redistribution among receptors (such as most foods) are not likely to exhibit spatial variability within a region; therefore information about percentage of the population that is exposed will be sufficient to quantify the receptor population.

Ideally a regional exposure assessment will represent the probable exposure of most of the local population for all times of the year and under all environmental conditions typical for the area. Since an assessment of this detail can be very difficult and costly to perform, especially if it requires the use of complex fate models, exposure estimates may be limited to average seasonal conditions (e.g., summer--

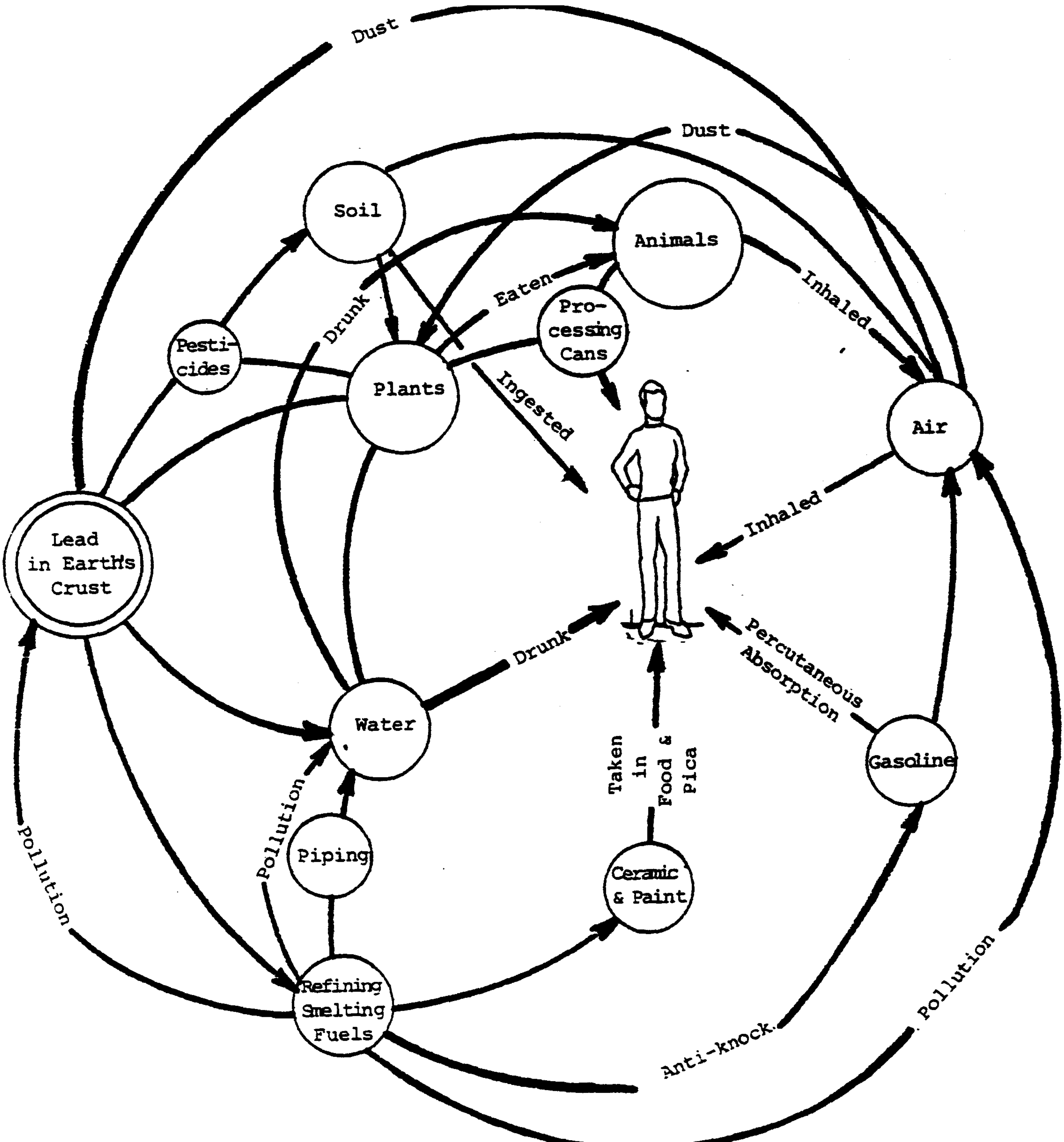


FIGURE 6-1: HUMAN EXPOSURE ROUTES - LEAD

Source: Perwak, J. et al. (1981).

low flow -- low rainfall, etc.) and to specific "worst case" meteorological or hydrological conditions for that area (e.g., 7 day-10 year low flow; no wind).

Chapter 5 described the algorithms used for calculating intake and the receptor population data needed to estimate exposure Chapters 3 and 4 described methods for the development of source and emissions data and for estimating pollutant concentrations in exposure media. Essentially the output of each task serves as input to the subsequent task. Qualitatively, information from each of the tasks also helps to define and refine the elements of other tasks. In anticipation of the eventual linkage of the tasks, the ways of expressing the data (units, time steps, etc.), especially input and output data, should be made consistent at the outset of a geographic study.

The following section describes a general methodology for conducting an exposure assessment, discusses the input requirements, and presents different ways to analyze and apply the results of the exposure assessment. The methodology is by no means uniquely correct, but is presented as a suggested framework for organizing regional exposure assessments.

6.3 METHODOLOGY

The Exposure Assessment can be roughly broken down into three general steps: organization of existing parameters and data and interface of models; calculation of individual exposure and population exposure levels; and analysis and applications of exposure data. Each step is discussed below in detail.

6.3.1 Organization of Input Parameters and Data

The input requirements for the regional exposure assessment are the following:

- pollutant concentrations in environmental media (described in Chapter 4)
- pollutant intake computational methods (Chapter 5)
- receptor population data (Chapter 5)

6.3.1.1 Pollutant Concentration Data

Pollutant concentrations are either in the form of monitoring data measured in the study region or estimated levels based on the predictions of fate model simulations of the area. For monitoring data, both mean or median and maximum values should be used in estimating exposure; the former as representative of an exposure typical of the majority of the population, and the latter as an upper limit on regional exposure. Monitoring data should be collected from sites at which exposure is likely to occur and the data should represent variability in pollutant loadings, as well as seasonal and other variability. Monitoring data from most regions, however, are usually limited, and the use of pollutant fate and transport models will undoubtedly be required to simulate pollutant concentrations in exposure media.

Two modelling approaches can be used to estimate pollutant concentrations. A multimedia fate model including transport of pollutants between and the fate and distribution in all environmental compartments is one method; however these models are often complex and expensive. Simpler single compartment models can also be implemented provided coefficients are included to estimate transport into important exposure media through processes such as deposition from air to ground and plants, uptake by plants from soil, uptake by livestock from water and feed. Both modeling approaches are discussed in the Environmental Pathways Analysis (Chapter 4).

6.3.1.2 Standard Fate Models

The model(s) selected in the Environmental Pathways analysis (Chapter 4) should be responsive to the requirements of the Exposure Assessment analysis; therefore, there should be initial input from the exposure team in the choice of models, boundaries, time-steps, location of receptor sites and other factors. From the point of view of the Exposure Assessment, fate models should :

- be sensitive enough so that exposure of near-field populations can be quantified;

- produce pollutant concentration estimates at reasonable time intervals so that exposure estimates can be expressed in a form compatible with health effects data;

- give pollutant concentration estimates within a bounded area and at spatial locations reflecting receptor distribution patterns;

- estimate concentrations representative of local pollutant release patterns, of average seasonal and worst-case meteorological conditions for the study region, and of the physical and chemical variability within each medium modeled.

In general, the final output of an environmental fate model will be a concentration or mass of pollutant in a volume or mass of environmental media, either at equilibrium or as a function of time. In some models, a concentration frequency distribution for a pollutant can be generated as a function of local environmental conditions, release patterns, or other variables. This distribution is useful in estimating the probability of exposure to different concentrations or in generating a realistic estimate of average and maximum exposures. For regional models, the spatial distribution of various concentrations or ranges within a specified bounded area can also be given.

6.3.1.3 Exposure Pathways Not Usually Considered in Fate Models

In a regional exposure assessment, it may be desirable to estimate concentrations in environmental exposure media not included in standard fate pathways models. The following briefly discusses some of these cases and possible approaches for their inclusion.

Home Gardens: Certain toxics accumulate in vegetables grown in urban home gardens or agricultural areas via uptake from contaminated soil (by fall-out at previous waste disposal sites, by soil erosion and transport from industrial sites), from atmospheric deposition, or from irrigation with contaminated water. If a soil/air intermedia model is implemented, then estimates can be made of soil concentrations at a particular site and thus, if the process of plant uptake of the chemical is understood, estimates of plant concentration can be developed. Also plant surface concentrations can be estimated from a rate of atmospheric deposition. The AIRDOS-EPA model for radionuclides describes a method for estimating plant uptake from deposition and soil. At this time, both types of estimates are uncertain for most toxic chemicals due to a lack of empirical data on plant uptake of these substances.

Fish: Most surface water models do not estimate pollutant concentrations in biota. The EXAMS model does include prediction of concentrations in phytoplankton but not in any species ingested by humans. The water column concentration output from these models can be used to roughly estimate tissue levels in fish if the equilibrium bioconcentration factor (BCF)* is known for that pollutant. The Criteria and Standards Division of the EPA, Office of Water, has estimated BCF's for many of the priority pollutants. These are published in the Criteria Documents; other data are also published in journals such as Environmental Health and Contamination, Residue Reviews, Journal of the Water Pollution Control Federation, Environmental Pollution, and others.

Drinking Water: In the absence of drinking water monitoring data, pollutant levels in surface water supplies may be estimated by retrieving ambient concentration data (e.g. from STORET) at locations upstream from the drinking water plant intake or, if available, at the intake itself. The effectiveness of the plant's treatment methods in removing any pollutants present in the influent can then be evaluated and predictions made of the

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* Ratio of fish tissue concentration to water column concentration.

pollutant concentrations at the tap. The STORET User Service or staff members of the Monitoring and Data Support Division can provide information on these methods. Pollutant levels in groundwater are more difficult to estimate. However, with the use of a soil pollutant transport and transformation model (such as SESOIL), the impact of a pollutant on the water quality of an underlying aquifer can be assessed if local soil conditions and geology are known and ground water concentrations estimated. For all types of water supplies, the rate of formation of chlorinated organics during chlorine treatment may be modeled if judged to be an important pollutant source for the area.

6.3.1.4 Linkage of Fate Models to Receptor Distribution Models

One of the problems likely to be encountered in a regional exposure assessment is the interface of the environmental fate models with receptor distribution models or exposure site data. The dimensions and bounds of fate models are usually dictated by local topography and meteorology and by emissions patterns. Population subdivisions are based on factors such as population density, political boundaries and sometimes natural boundaries. Ideally, an a priori methodology should be decided upon in order to systematically coordinate these two sets of data. The methodology will be determined by the type of fate model employed.

The output of a compartment box model, such as EXAMS, is an average concentration for a specified area. In the initial decision-making concerning model bounds, the location of exposure sites should be accounted for to ensure their placement within model compartments rather than straddling boundaries. For atmospheric box models, which are likely to have too few boxes to accommodate the desired number of Census Bureau divisions, the interface may be more difficult. At least two options are available:

- the initial division of the study area into model boxes may be based on census bureau delineations, so that one fate box is equivalent to a population district or some fraction of a district.
- Fate box boundaries may be determined independently from population data. Subsequently, populations within these box areas may be estimated from census bureau and land use data. There would be a greater uncertainty associated with using these estimates instead of directly using census bureau district populations.

Additionally there may be other approaches developed by government agencies involved in atmospheric exposure modeling, such as EPA's office of Air Quality Planning and Standards.

Gaussian plume models generally report concentration output at predetermined locations or receptor points. The placement of one set of receptor points should largely be the responsibility of the exposure team and be based on population trends. For example, a single receptor point may be specified for small census bureau divisions such as city blocks. Larger divisions, such as enumeration districts, may require several receptor points; the concentrations reported at these points may be averaged or weighted and averaged to give a mean level for the districts. It may be important to locate receptor points at specific sites with a high population density or sensitive locations such as apartment complexes or hospitals. These receptor points may represent at the same time, depending on their location, the census bureau district in which they are found.

6.3.1.5 Occupational Exposure

For certain toxics, workplace exposure may be more significant in terms of magnitude of pollutant intake levels than is environmental exposure. For example, exposure levels resulting from dermal absorption or inhalation of substances like chlorinated solvents and pesticides may be two or more orders of magnitude greater than the levels to which the general, non-occupational population is exposed. In a geographic exposure assessment, which predominantly uses very detailed and localized information, it may be important to estimate the occupational exposure of the human receptor population in order to place the environmental contribution to total exposure in a better perspective. For instance, there may be a geographic area in which the majority of the work force is employed by a major industry with high on-site airborne concentrations but low atmospheric emission rates. If exposure outside of the workplace is negligible compared to occupational exposure, then emission controls may do little to reduce exposure to an acceptable level, and control strategy development should address reduction of onsite levels. In addition, there may be a trade-off between occupational and environmental exposure. For example, increasing ventilation inside a plant to reduce employee exposure may increase the exposure of the general population living downwind from the site. Therefore, information on the exposure levels and number of receptors associated with each exposure pathway would be required to select and evaluate the most effective control strategy for this situation.

Occupational exposure assessments have been primarily conducted by the Occupational Safety and Health Administration (OSHA) and the National Institute of Occupational Safety and Health (NIOSH). The assessments are usually based on extensive on-site monitoring data and not on model predictions. Certain offices within the EPA, such as the Office of Presticide Programs and the Office of Radiation Programs, may also estimate occupational exposure. The present methodology does not attempt to describe or evaluate the various approaches used in estimating occupational exposure. In a geographic exposure assessment requiring occupational exposure information, the first step would be to contact the organizations listed above and other relevant groups (e.g. the state, industry organizations) for specific approaches and information.

6.3.2 Calculation of Individual and Population Exposure Levels

Once the input data and computational algorithms are organized and the interfaces between fate and exposure models completed, the exposure calculations can be made. Exposure levels are calculated for each exposure pathway (e.g., dermal absorption from surface water) and for each subpopulation or subregion (e.g., swimmers at a beach immediately downstream of an effluent pipe) designated for that pathway. The results of the exposure calculations can be expressed in at least two different ways:

- typical or maximum individual intake (e.g., µg/day of pollutant)
- population intake or population exposure factor (e.g., µg/day of pollutant multiplied by population exposed)

Intake is presented as a rate, usually as a daily, seasonal or annual exposure. The selected time frame is determined by the intended application of the exposure results (e.g., whether they are to be used in assessing the health impact of acute or chronic exposure), a decision which is, in turn, a function of the particular pollutant's emission, fate, toxicological and exposure characteristics. For example, long-term exposure to an intermittently released pollutant with a short environmental half-life (e.g., a haloether) will be of less relevance than exposure to a relatively persistent pollutant (e.g., a chlorinated hydrocarbon). In the latter case, annual exposure will be important to quantify.

These results can be presented in tabular or graphic form, broken down by exposure pathway or subpopulation. Table 6-1 is an example of

TABLE 6-1

SUMMARY OF INDIVIDUAL INTAKES AND POPULATION EXPOSURE FACTORS FOR THE FOUR STUDY POLLUTANTS[1]

	Chloroform	Vinyl Chloride	Carbon Tetrachloride	Lead
DRINKING WATER CONSUMPTION				
individual intake (μg/day):	120-180	NE[2]	NE	<30
maximum population exposure factor (μg/day · population / 1000)	Not calculated based on prelimi-nary data	NE	NE	Not calculated based on limited data.
FISH CONSUMPTION				
individual intake (μg/day): mean/max.	0.02/5.3	0.0001/0.02	0.05/15	9.6/580
population exposure factor (μg/day · population / 1000)	0.8	0.04	1.6	343
HOME PRODUCE CONSUMPTION				
individual intake (μg/day): range	NE	NE	NE	0.06-1.0
population exposure factor (μg/day · population / 1000)				4.1-6.8
SURFACE WATER ABSORPTION				
individual intake (μg/day): mean	15	2×10^{-4}	5×10^{-3}	0.02
population exposure factor (μg/day · population / 1000)	<0.01-0.4	<0.1	<0.1-0.2	<0.1
AIR INHALATION				
See Table 5-31.				

[1]Assumptions for these values are given in the preceding study.

[2]NE = Not estimated due to lack of data.

Source: Kanawha Valley Regional Exposure Assessment. July, 1981.

one method of presentation. For exposure pathways which have regional differences, e.g., inhalation of air, exposure levels may be graphed to illustrate their relationship to sources or local topography. Figures 6-2 through 6-4 illustrate a means of displaying these data for a specific area.

The level of detail to be used in the breakdown of regional subpopulations will depend on the sensitivity of the model and the environmental behavior of the pollutant. For example, it may be possible to aggregate regional receptor subpopulations into larger and larger groups with increasing distance from an atmospheric source due to a concurrent decrease or stabilization in pollutant concentration. Usually, a preliminary fate model run and sensitivity analysis is required before it is possible to make these decisions regarding elimination of receptor points.

6.3.3 Analysis of Exposure Data

Receptor populations are likely to be exposed to toxics through more than one exposure pathway at a time. Therefore, individual exposure levels may be combined into a total exposure for intake of a pollutant through ingestion of different substances, dermal absorption from surface water and water supply, and inhalation at different locations in the study area (e.g., work, recreational areas, home, commuting routes). If the pharmacokinetics of absorption for each route are understood for the pollutant being modeled, then these different exposure can be aggregated into a single total exposure. Otherwise the exposures for each route must be presented separately and compared.

Daily and annual exposure profiles or scenarios can then be developed for various subpopulations in the study area. The subpopulations selected

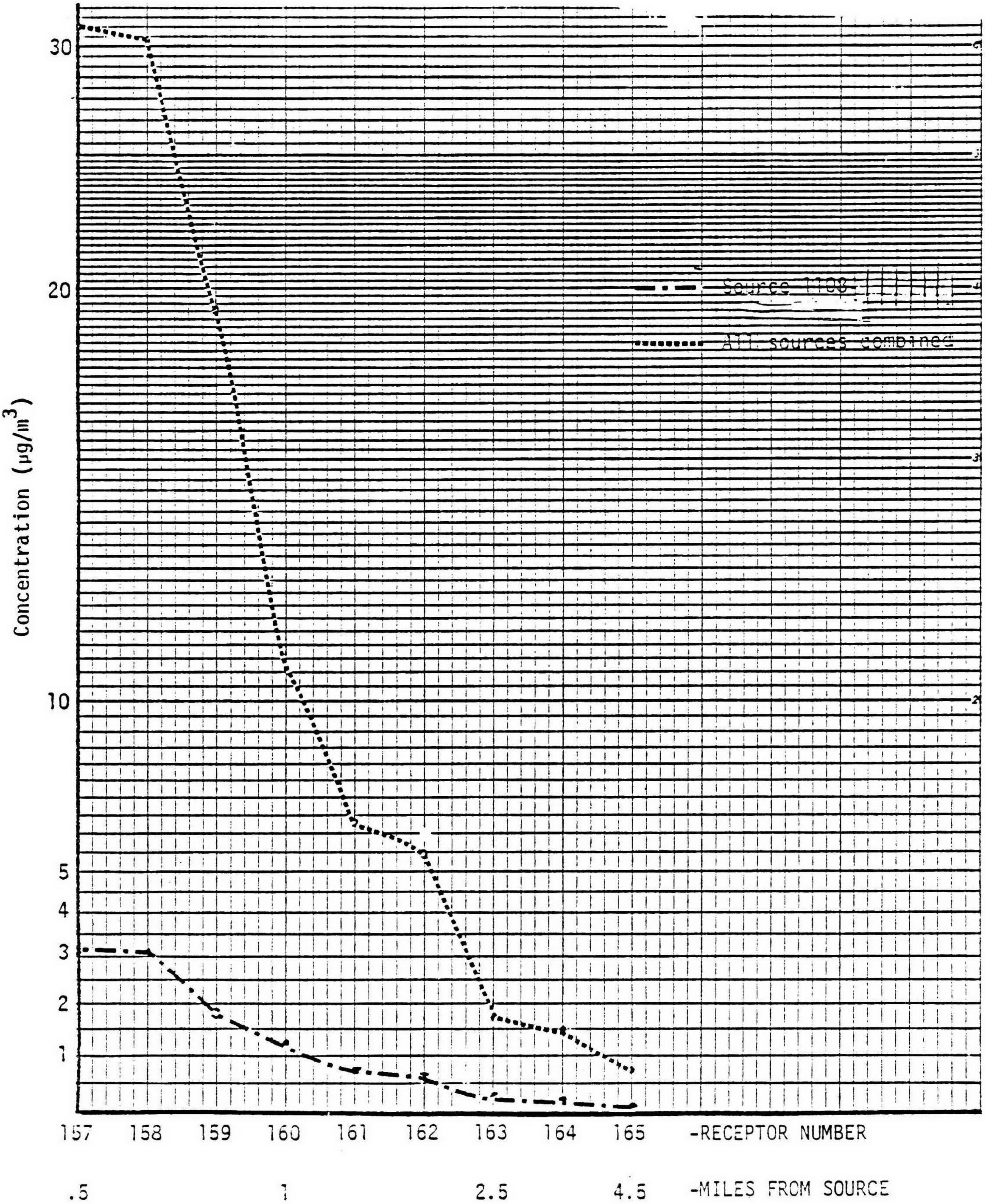

FIGURE 6-2 RELATIONSHIP BETWEEN SAMPLE POLLUTANT CONCENTRATION AND DISTANCE FROM SOURCE

SOURCE: A.D.L. (1981)

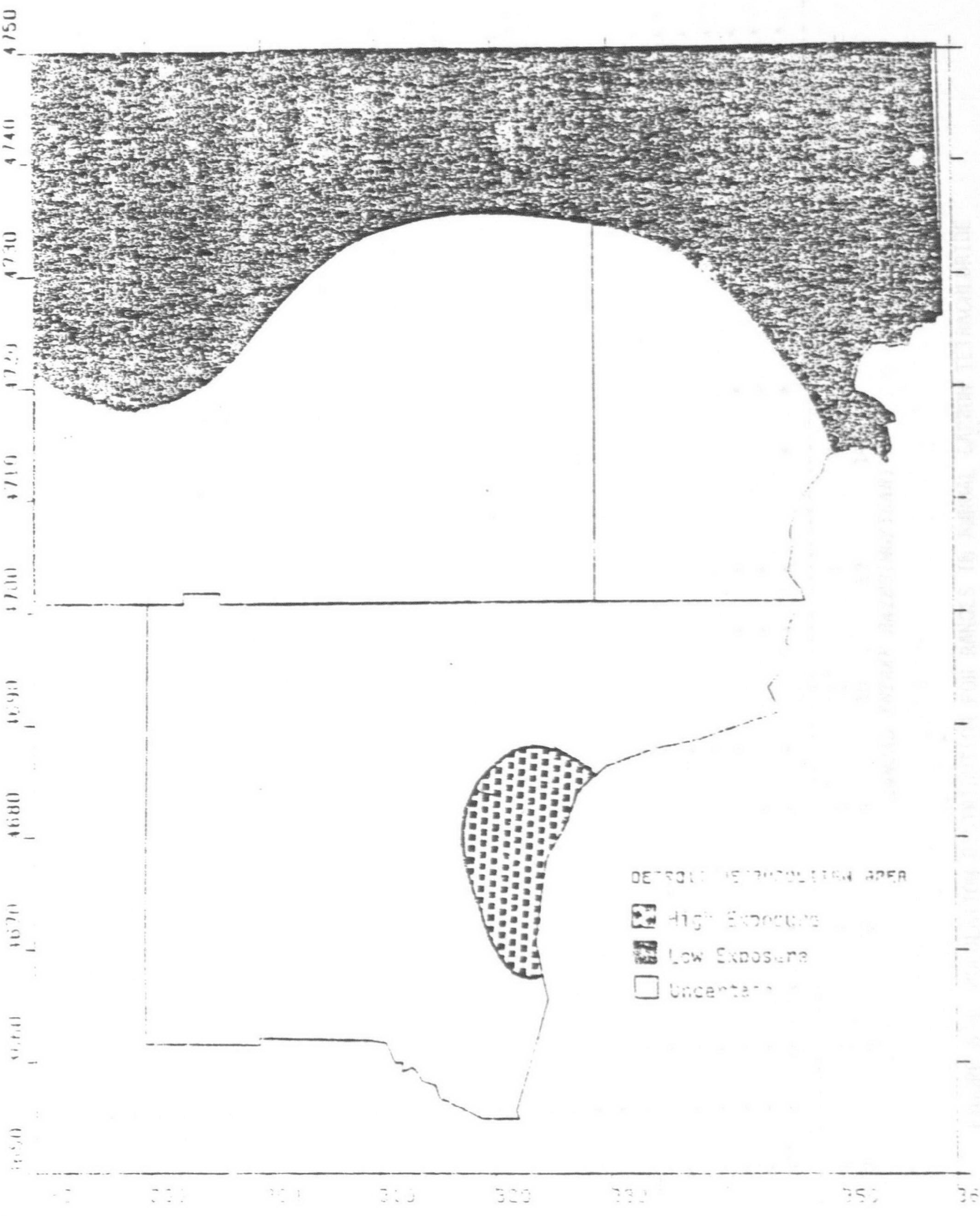

FIGURE 6-3: EXPOSURE CHARACTERISTICS OF NICKEL EMISSIONS

Source: NAGDA 1979.

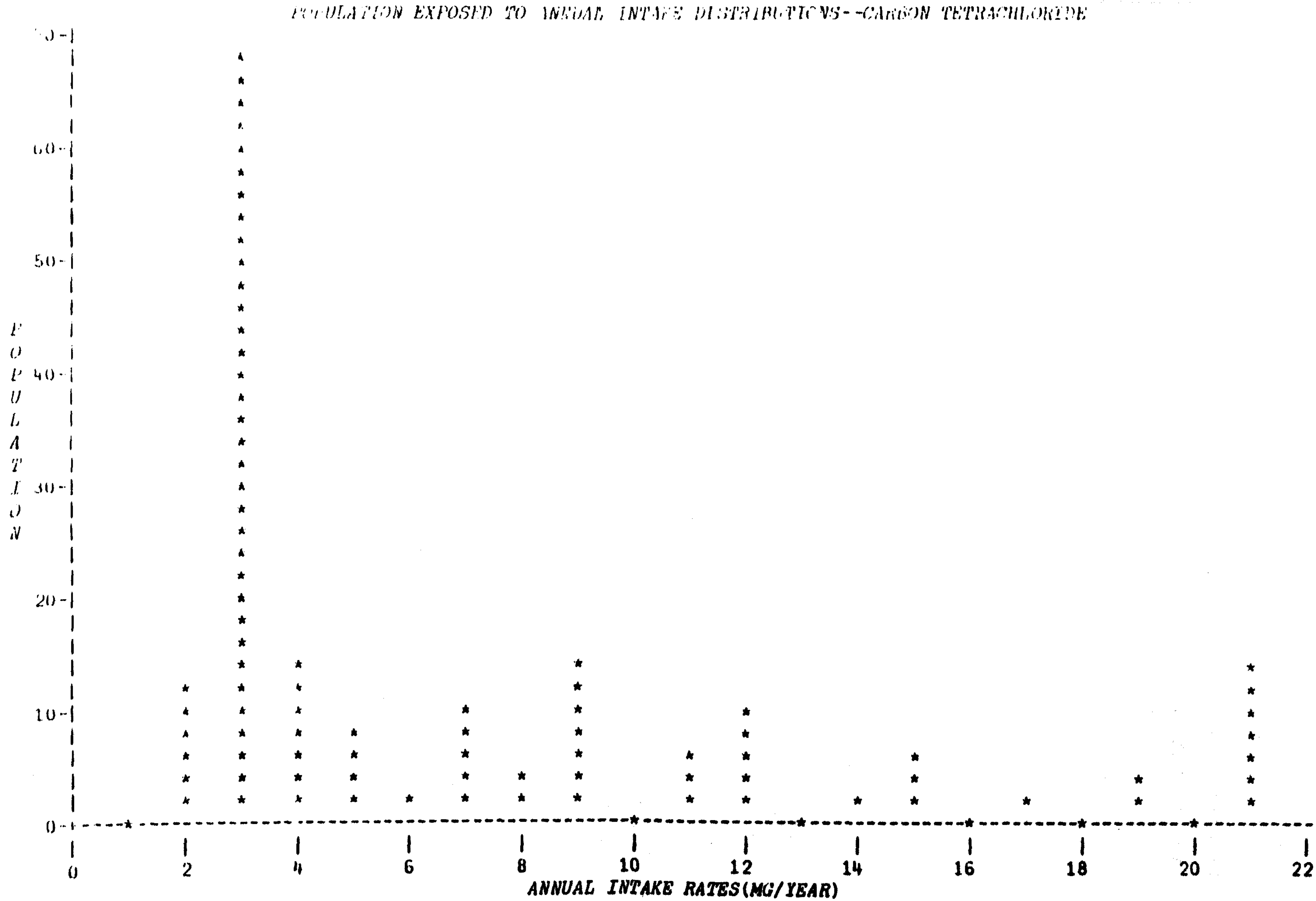

FIGURE 6-4 POPULATION DISTRIBUTION FOR RANGES IN ANNUAL CARBON TETRACHLORIDE INTAKE RATES

will depend on the characteristics of the study area, e.g., recreational use, presence of agriculture, transportation patterns, climate, etc. Some examples for humans of possible scenarios include:

- typical exposure for the general population by sex, age group
- occupational exposure
- commuters
- users of certain home products
- summer vs. winter exposure
- recreational exposure
- exposure of residents in the vicinity of a hazardous waste disposal site.

6.4 APPLICATIONS OF EXPOSURE ASSESSMENT RESULTS

The estimates of regional human exposure by route and subpopulation can be used directly, without comparison to health effects data, in a number of applications to evaluate potential toxics problems in an area.

- Comparison of regional exposure levels to national "average" exposure levels;
- Comparison of the impact of different routes or pathways of exposure such as drinking water vs. inhalation;
- Comparison of locally attributable exposure vs. imports from outside (such as in foods);
- Comparison of daytime to nighttime exposure or identification of seasonal variability in exposure;
- Comparison of source-proximate (near-field) subpopulations to the rest of the population (far field);

- Identification of the regional toxics source(s) responsible for the greatest exposure, both in terms of population affected and magnitude of individual intake;
- Preliminary identification of large or sensitive subpopulations or high-exposure areas in the region;
- Comparison of exposures to different pollutants released by the same sources or through the same environmental media.

Another potential application of the human exposure data developed for a specific region will be to evaluate the impact of the exposure levels in terms of health risk. The more detailed the exposure analysis, the more accurately is an assessment of risks associated with regional exposure. Human health data may be specific to selected subpopulations or conditions (such as dosing) so that the level of detailed required in the exposure assessment may include population breakdown by age, sex, race, as well as other groups such as pregnant women, people with respiratory ailments, and so forth. The exposure estimates should reflect individual dosage over small time steps and the cumulative dose at any time, as well as the duration of exposure, fluctuations in dosing, and perhaps, presence of and interactions with other substances and other influential factors. However, the precision obtained through much exposure estimation may be more than outweighed by the uncertainty associated with health effect estimates, particularly in the case of low-dose extrapolation (e.g., for carcinogenesis).

6.5 REFERENCES

Arthur D. Little, Inc., A Pilot Study - International Commission on Radiological Protection (ICRP). Report of the task group on reference manual, Oxford, England: Pergamon Press; 1975.

Arthur D. Little, Inc., Integrated exposure/risk assessment methodology. Preliminary draft. Contract 68-01-3857. Washington, D.C.: Monitoring and Data Support Division, U.S. EPA; 1980.

Consumer Product Safety Commission (CPSC) as cited in U.S. EPA; 1980.

Food and Drug Administration (FDA). Total diet studies. Compliance program evaluation. Washington, D.C.: Bureau of Foods; 1973 and 1980.

Moore, R.E., Baes, C.F., McDowell-Boyer, L.M., et al. AIRDOS-EPA: A Computerized methodology for estimating environmental concentrations and to man form airborne releases of radionuclides. EPA 520/1-79-009. Washington, D.C.: Office of Radiation Programs, U.S. Environmental Protection Agency; 1979.

Navada, N.L. Environmental carcinogens and human cancer: estimation of exposure to carcinogens in the ambient air. EPA 600/1-79-002. Research Triangle Park, NC: Office of Research and Development, U.S. Environmental Protection Agency; 1979.

Perwak, J. et al. Exposure assessments of priority pollutants: Lead. Interim Draft. Contract EPA 68-01-3857. Washington, D.C.: Monitoring and Data Support Division, Office of Water Planning and Standards, U.S. Environmental Protection Agency, 1980.

Pielou, E.C. An introduction to mathematical ecology - Toronto: Wiley-Interscience; 1969.

Pollard, J.H. Mathematical models for the growth of human populations. Sidney, Australia: Macguarie University, Cambridge athe the University Press; 1973.

United States Department of Agriculture (USDA). Food and nutrient intakes of incividuals in the United States. Washington, D.C.: Agricultural Research Service; 1980.

U.S. Environmental Protection Agency. The exposure assessment group's handbook for performing exposure assessments. Preliminary draft, not formally released by EPA. November, 1980.

U.S. Environmental Protection Agency. Identification and evaluation of waterborne routes of exposure from other than food and drinking water. EPA 440/4-79-016. Washington, D.C.: Office of Drinking Water, U.S. Environmental Protection Agency; 1979.

U.S. Environmental Protection Agency. Proceedings of Workshop on Exposure/Assessment of Hazardous Chemicals, as cited in U.S. EPA 1980. By Radian Corporation, EPA contract No. 68-02-3171; 1980.

8. PRACTICAL CONSIDERATIONS

8.1 FEASIBILITY OF THE GEOGRAPHIC APPROACH

From a technical point of view, the geographic approach allows the use of detailed local information to arrive at highly specific conclusions regarding toxic substance multi-media problems, and then permits the development of appropriate control strategies. This approach is feasible provided that sufficient data are available in the various pathways of concern. In some cases, a preliminary data-gathering and field sampling program may be necessary in order to lay the groundwork for a geographic study. In other cases, the need for additional data may be recognized only after a first iteration of the exposure assessment methodology. Apart from the problem of data sufficiency, the other elements of the geographic approach have a sound technical basis. Though there is some uncertainty with regard to the outputs of fate and transport models, as well as exposure models, these outputs provide a sufficient degree of resolution to permit control strategy development.

A geographic study, especially in the control strategies development task, will require special administrative coordination so that representatives from relevant Federal, State and local programs and interest groups can have access to the on-going work. Some routine forums, or ad hoc tasks forces may be required to provide continuing interaction among these parties. Public relations offices in each agency will have to provide some of this coordination.

More importantly, means of communicating interim study results to relevant parties will be very important in promoting meaningful inputs from these parties, especially where control strategies other than command/control are introduced. Similarly, means of soliciting inputs from affected groups, industry, commercial, local authorities or community groups will be essential if a working cooperation is to be pursued. The Federal EPA can provide much needed guidance in this area.

The most difficult administrative problems for control strategies development are likely to be associated with managing local problems through local authorities. Here, the amount of technical expertise required to provide input on assessments of the technical feasibility of alternative control options will be quite high due to the site-specific nature of such issues. If many studies are under way, the agencies may have a critical deficit of such expertise available either in-house or through its contracted services. This shortage of technical expertise will affect not only the problem diagnosis and control strategy selection phase but also the follow-up program phase. It may be advisable in some cases to consider developing a stock of locally available expertise. In such a case, some local people with interest and relevant professional background or experience might be brought into the study project and prepared to manage some of the required follow-up programs. Such a group could at the minimum serve as an interface between the study project and continuing efforts to implement resulting controls. This prospect, however, could introduce another layer of administrative complexity, and the efficiency of such a strategy should be explored.

8.2. POTENTIAL LIMITATIONS OF THE METHODOLOGY

8.2.1. Adequacy of Data

The most important limitation that will be encountered in any future implementation of the geographic approach is the adequacy of the available data. This particularly affects the inventory of sources and emissions, which is the foundation of the entire exposure assessment methodology. Development of quantitative emission estimates on a source-specific basis requires detailed information which simply may not be available. The use of assumptions, approximations, or national averages to characterize emission rates can be a useful approach, but will tend to weaken the credibility of the results. There is no unified set of default values that may be used in the absence of specific data. Moreover, there will inevitably be gaps in the identification of pollution sources, due to non-uniform reporting practices and ongoing changes in the study area. New facilities or modifications in old ones may not be recognized, and existing records may omit certain critical items of data. The source categories for which data gaps are expected to be most acute are as follows:

- hazardous waste disposal
- toxics emissions to air
- non-point loadings to surface water
- point source discharges to water for industries other than the primary ones or for non-priority pollutants.

Information for the source emissions quantification will rely mainly on data furnished by industries in compliance with regulatory requirements; as these requirements change, the data base will vary accordingly. In general, it will not be possible to provide frequency distributions for source emissions. The level of precision will usually be confined to point estimates and ranges of variation, thus limiting the statistical accuracy of the subsequent exposure assessment tasks.

Inadequacy of data can limit the accuracy of the exposure assessment in other ways. The absence of sufficient field monitoring data for air, water, soil, or biota can make it more difficult to analyze environmental pathways for toxic pollutants and to validate the results of modelling efforts. Since modelling can only be performed for selected pollutants and selected media, an exposure assessment must rely upon monitoring data to ascertain the ambient levels of many of the pollutants under consideration. Furthermore, the estimation of exposure levels for specific receptor groups requires a considerable amount of data concerning recreational patterns, dietary habits, and population distribution, which may be scarce or nonexistent. These types of data gaps will result in exposure estimates that may be incomplete for certain substances in certain media, or that may have high levels of uncertainty.

Finally, in the control strategy development phase, the data problems indicated above will often make it difficult to present credible quantitative conclusions for the purpose of justifying exposure problems or the need for control options. In some cases it may not be possible to establish a substantial link between sources and receptors upon which environmental benefits must be predicated. However, even when the environmental pathways are well understood, there are additional data concerns which may limit the usefulness of the control strategy analysis. For example, the costs and efficiencies of emission controls will often be difficult to evaluate on a site-specific basis, due to confidentiality restrictions and peculiar features of individual facilities. Cost estimates based on generic industry data may distort considerably the actual situation in the study area.

8.2.2. Validity of Models

A critical link in the exposure assessment methodology is the analysis of environmental pathways of toxic substances. Therefore, an important limitation of the general methodology has to do with the limitations of the single medium models to be employed. In general, these limitations may be due to: (1) data availability, (2) inappropriate model selection, (3) omission of important pathways, and (4) lack of appropriate model validation.

The types of data required for pathway modelling include environmental data (e.g., pollutant import to basin), chemistry data (e.g., chemical properties of pollutants) and monitoring data (e.g., ambient concentrations). (The latter was discussed in Section 8.2.1.) It is not appropriate, for example, to drive any river model without a proper set of flow records, nor to attempt validation of the model output with inadequate monitoring data.

With regard to model selection, the choice of a single medium model requires a compromise between level of sophistication, data availability, and needs and resources (computer, time, budget) of the project. Selecting for example, a numerical finite element groundwater model and a lump-sum simulation watershed model might be an inappropriate decision due to mathematical complexity and pragmatic difficulty. The selected models will inevitably require some simplifying assumptions such as complete mixing in rivers or average long-term meteorological conditions. Omitting certain important pathways (e.g., waste disposal site to groundwater to river) because of lack of data may also be an issue of concern. Such pathways should preferably be discussed, and perhaps modeled with simplified algorithms, so that their omission can be justified.

Finally, model calibration and model validation are an important part of the general methodology application. Non-validated modelling efforts can have only qualitative use; therefore, final model predictions should be validated with any available data. However, a disagreement in absolute levels does not necessarily indicate that the selected method was incorrect or that data sets employed are suspect. Rather, it indicates need for recognizing the methodology limitations and for performing sensitivity analyses upon the data sets in question. Engineering judgment and professional experience will be required to assess the range of uncertainty in model predictions and the importance of discrepancies between those predictions and monitoring data.

8.2.3. Scope of Analysis

An important limitation of a geographic study may arise from the scope under which the study is conducted. The present methodology has selected exposure as a quantifiable endpoint of the analysis; thus health effects of pollutant exposure have been excluded from scope. Since healt effects are not site-specific, it can be argued that information about health and environmental imports could be incorporated with the results of the geographic study in order to assess the benefits of various control strategies. However, consideration of health effects as an independent item of information implies that exposures will not be weighted according to the relative potency or severity of effects for different pollutants.

Though toxicity was considered in the pollutant selection (Section 2.3), the subsequent exposure assessment and control strategy analysis did not explicitly address the different risks associated with the pollutants in question. Unfortunately, the present state-of-the-art of risk assessment does not permit accurate quantification of risk; in fact, the only effect for which quantitative estimates of risk are possible is carcinogenesis, and even in this case the range of error is enormous. Thus the inclusion of risk estimates would greatly decrease the accuracy and credibility of the results. Moreover, explicit statements about risk to local populations might be inflammatory and could create unnecessary difficulties for Federal and State authorities by suggesting unconfirmed problems.

Another potential limitation associated with the scope of the study is the variety of possible exposure routes that are considered. The present methodology has focused heavily upon exposure to toxics in the ambient environment, including food and drinking water, but has paid little or no attention to exposures that may arise in occupational, commercial, or residential settings. This emphasis is due mainly to the limits of the EPA's jurisdiction. However, the total exposure of individuals to a particular toxic substance may be an important criterion in the development of regulatory strategies. For example, if only 5% of average per capita exposure to a substance is due to environmental pathways, then reduction of environmental emissions by 90% will have an inconsequential effect upon the per capita risk associated with that substance. Thus, a broader scope of analysis may be warranted, if only to gauge the true significance of environmental emissions. It might be advisable for the EPA to coordinate with other Federal agencies, such as OSHA or FDA, in the context of the geographic approach, so that a more complete perspective is obtained concerning toxic substance exposure.

8.3. STUDY TIMETABLE AND RESOURCE REQUIREMENTS

The general methodology outlined in this report has focused upon the functional activities required to perform a geographic study. Administrative questions such as staffing, public relations, and division of authority have not been dealt with here. From a purely technical point of view, however, it is possible to lay out a master project flow chart, showing the timing and relationships of the various activities described in the previous chapters. This chart is displayed in Figure 8-1. The three main phases of a geographic study are depicted with dotted lines, as defined in Section 1.4. In addition, the interaction between a field sampling program and the study tasks is shown. The EPA has had extensive experience in designing such sampling programs, so that the incorporation of field work into the geographic study will present no hidden technical obstacles. It is anticipated that the field work could be performed in parallel with Phase 2 of the study, creating little or no time delay. Modifications to the study outputs based upon field results could normally be incorporated toward the end of Phase 2. However, if the field work produces some surprise results which alter the significance of certain environmental pathways, some revision of the initial scan and exposure assessment scope might be required. In a situation where the initially available data were totally inadequate, it might be advisable to perform the field work prior to completing the initial scan. In such a case, the indicated parallelism would not be possible, and the duration of the study would be extended by as much as nine months.

The anticipated requirements of a geographic study in terms of professional time, computer and other expenses, and calendar time have been estimated in very rough terms. These estimates are shown in Table 8-1; note that field sampling cost estimates, though they have not been included, could easily exceed the costs of the study itself. Because of the variability in potential site characteristics, and because of the limited experience to date (only one pilot study), it must be recognized that actual costs could differ considerably from these estimates. They are

FIGURE 8-1: Activity Flow Chart for Geographic Study

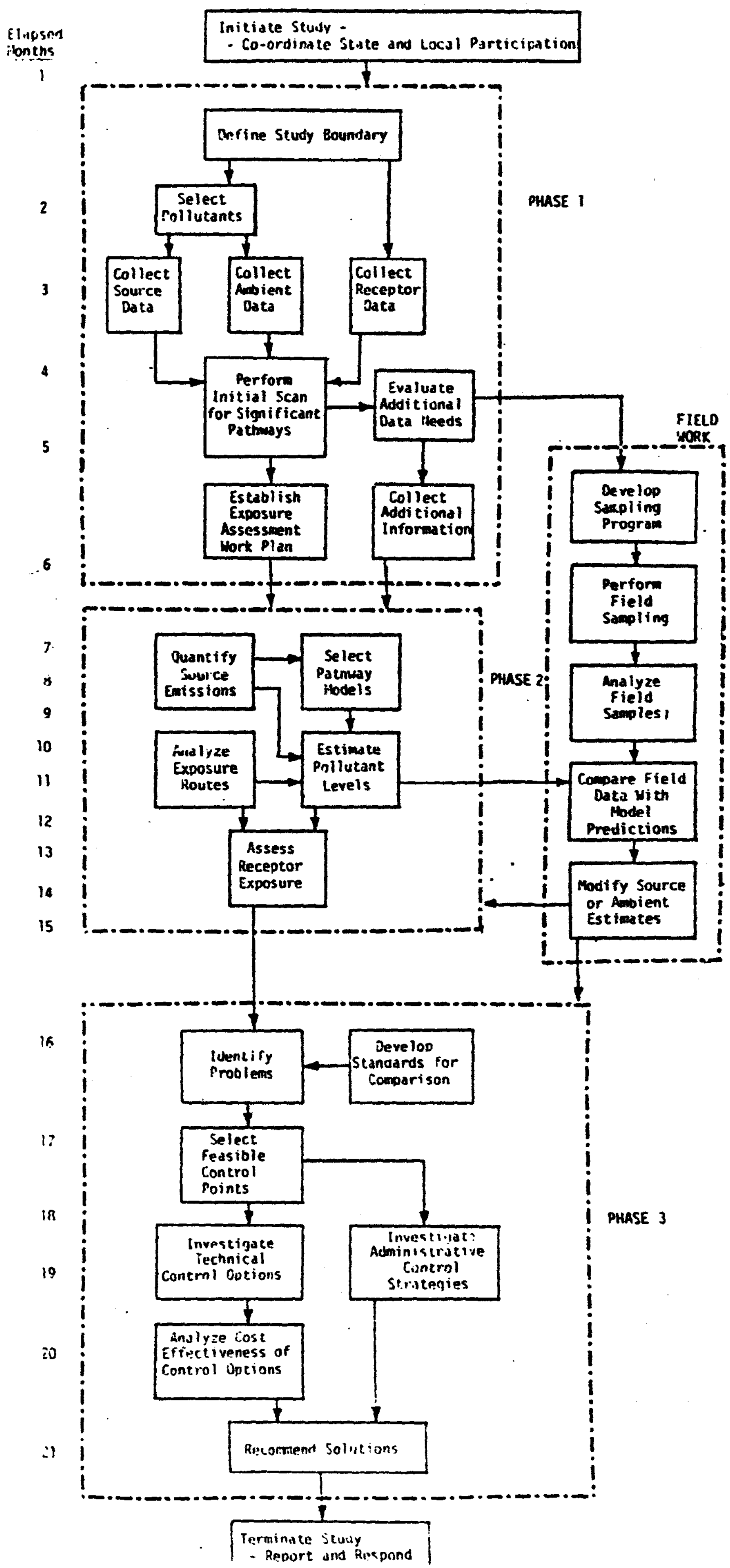

TABLE 8-1

ESTIMATED RESOURCE REQUIREMENTS FOR A GEOGRAPHIC STUDY
EXCLUDING FIELD SAMPLING

		20 POLLUTANTS			40 POLLUTANTS		
PHASE	TASK DESCRIPTION	Professional Time (Man-Hours)	Expenses including Computer)	Duration (Months)	Professional Time (Man-Hours)	Expenses including Computer)	Duration (Months)
1	State and Local Coordination	200		1	200		1
	Boundary Definition	200		**	200		**
	Selection of Pollutants	400		1	400		1
	Data Acquisition	2,000		**	2,000		**
	Initial Scan of Pathways	1,000		3	1,000		3
	Phase 2 Planning	200		1	200		1
	PHASE 1 TOTAL	4,000	$20,000	6	4,000	$20,000	6
2	Management and Reporting	1,000		**	1,000		**
	Source Identification	500		1	500		1
	Quantification of Emissions	1,500		2	2,500		2
	Pathway Analysis*	4,000	$20,000	4	6,000	$40,000	4
	Receptor Analysis	1,000		**	1,000		**
	Exposure Assessment	1,000		2	2,000		2
	PHASE 2 TOTAL	9,000	$40,000	9	13,000	$60,000	9
3	Management and Reporting	1,000		**	1,000		**
	Problem Identification†	500		1	1,000		1
	Selection of Control Options	1,000		2	2,000		2
	Evaluation of Control Options	2,000	$10,000	2	3,000	$20,000	2
	Strategy Development	500		1	1,000		1
	PHASE 3 TOTAL	5,000	$25,000	6	8,000	$35,000	6
	GRAND TOTAL	18,000	$75,000	21	25,000	$105,000	21

† for one quarter of the pollutants

* for half of the pollutants

**can proceed in parallel with other tasks provided only as a guideline, subject to refinement as the geographic approach continues to evolve. Two different estimates are given, assuming that 20 and 40 pollutants are treated; clearly there are economies of scale in the latter case. Personnel requirements are expressed in man-hours, so that different conversion factors can be applied for cost estimation. In both cases (20 and 40 pollutants) it is assumed that pathway modelling is performed for half the pollutants addressed; this may be somewhat high, since in many cases either the necessary data may be absent or the priorities established may dictate a smaller modelling effort. Likewise, in Phase 3 it is assumed that the number of problems identified for further study is one-quarter of the total number of pollutants; this assumption is fairly arbitrary since actual occurrence of problems is difficult to predict. The duration of both options is the same under the assumption that increased man-power would be available for the 40-pollutant case. The size of the project team could vary, but if full-time people were assigned, about eight people would be required for the 20-pollutant case and about twelve for the 40-pollutant case. The mix of personnel is assumed to be about 20% managerial, 60% technical/scientific, and 20% clerical/support.

8.4 CONCLUSIONS

A geographically-oriented exposure assessment methodology has been developed which is suitable for the evaluation of intermedia toxics problems, and provides a basis for the development of cost-effective control strategies. Focusing on a well-defined local area permits a detailed inventory of sources and pathways of toxics exposure across all environmental media. Moreover, the investigation of feasible control options can include state or local authorities in seeking the most efficient solution to an existing or potential problem. Implementation of the geographic approach will require the development of an appropriate site selection mechanism for identifying local areas that merit this type of intensive investigation.

The general methodology consists of three phases of work: an initial scan period during which data are collected and priorities are established, an exposure assessment phase during which detailed technical analysis is performed of receptor exposure to selected toxics, and a control strategy phase during which means are sought for reducing specific exposure levels. Although the methodology is oriented toward quantification of exposure rather than risk, it would be a simple matter to extend the analysis by attaching risk estimates to each exposure level. However, such risk estimation may introduce a substantial amount of uncertainty, due to the difficulty of predicting human responses based on laboratory animal health effects data.

The key to successful application of the geographic methodology is the establishment of links between source emissions and receptor exposures, via a description of the environmental fate and pathways of toxic substances. This goal may be hampered by the absence of sufficient data or by the difficulty and expense associated with pathway modeling. However, explicit quantification of these links can provide a firm, rational basis for decision-making relative to alternate control strategies. Even when the source-pathway-exposure chain is not completely understood, a systematic identification of optional control mechanisms will permit a thorough evaluation of the costs and potential benefits of controlling the substances in question.

APPENDIX A -- POLLUTION FLOW MODEL

In a geographic study, the relationship between source emissions and ambient levels of toxic substances can initially be investigated through the use of environmental pathway models. However, for repeated sensitivity analyses these computer models become unnecessarily expensive to run. Instead it is possible to take advantage of the linearity in the model results, and to replace the computer simulation with a set of algebraic equations that relate emissions to ambient levels. This approach not only reduces the cost of multiple analyses, but also permits the determination of required emission levels as a function of target ambient concentrations. A summary of the algebraic approach is presented below:

Suppose the area of study consists of N well-defined cells, or regions, into and out of which a pollutant may flow. Suppose there are M sources of the pollutant in the area of study, each source contributing a fixed mass of pollutant (perhaps zero) to each cell in each time step. Suppose further that the proportion of the pollutant present in a given cell at the beginning of a time step which has flowed to another cell by the end of the time step is constant.

Define:

$$X(i) = \begin{bmatrix} x_1(i) \\ x_2(i) \\ \vdots \\ x_N(i) \end{bmatrix}, \quad x_j(i) = \text{mass of pollutant contained in cell } j \text{ at the beginning of time step } i.$$

$$A = \begin{bmatrix} \alpha_{1,1} & \alpha_{1,2} & \cdots & \alpha_{1,N} \\ \alpha_{2,1} & \alpha_{2,2} & \cdots & \alpha_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{N,1} & \alpha_{N,2} & & \alpha_{N,N} \end{bmatrix}, \quad \alpha_{i,j} = \text{proportion of mass in cell } j \text{ at beginning of time step that flows to cell } i \text{ by end of time step.}$$

$$U = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_M \end{bmatrix}, \quad u_i = \text{mass of pollutant discharged by source during one time step.}$$

$$B = \begin{bmatrix} \beta_{1,1} & \beta_{1,2} & \cdots & \beta_{1,M} \\ \beta_{2,1} & \beta_{2,2} & \cdots & \beta_{2,M} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{N,1} & \beta_{N,2} & & \beta_{N,M} \end{bmatrix}, \quad \beta_{i,j} = \text{proportion of mass discharged from source j that is discharged into cell i.}$$

It follows, from our assumptions and these definitions, that the mass of pollutant contained in each cell at the beginning of time step n is given by:

$$X(n) = AX(n-1) + BU.$$

After many time steps, the mass of pollutant in each cell will be great enough so that the constant proportion flowing out will equal the proportions from other cells flowing in plus the fixed amount being discharged to the cell directly. The mass of pollutant in each cell will remain constant; the system has reached a steady state $\bar{X}$:

$$\bar{X} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_N \end{bmatrix}, \quad \bar{x}_i = \text{steady-state mass of pollutant in cell i.}$$

It follows that:

$$\bar{X} = A\bar{X} + BU,$$

$$\bar{X} = [(I-A)^{-1}B]U \tag{1}$$

where I is the identity matrix. Given proportions $\alpha_{i,j}$ and $\beta_{i,j}$ and discharges u_i, therefore, we may calculate the steady-state $\bar{X}$ directly.

Alternatively, we may calculate the quantity BU given a "target" $\bar{X}$:

$$BU = (I-A)\bar{X} \tag{2}$$

The quantity BU, it may be seen, gives the total mass discharged into each cell by all sources:

$$BU = \begin{bmatrix} \beta_{1,1}u_1 + \beta_{2,1}u_2 + \cdots + \beta_{N,1}\, u_N \\ \beta_{1,2}u_1 + \beta_{2,2}u_2 + \cdots + \beta_{N,2}\, u_N \\ \vdots \\ \beta_{1,N}u_1 + \beta_{2,N}u_2 + \cdots + \beta_{N,N}\, u_N \end{bmatrix}$$

Simple River Model

For a simple river model, we have:

$$x_i(n) = \alpha_{i,i}x_i(n-1) + \alpha_{i,i-1}\, x_{i-1}(n-1) + u_i.$$

That is, the mass of pollutant in cell i at the beginning of time step n is the amount remaining from the beginning of time step (n-1), plus the amount flowing in from the cell upstream, plus the amount discharged directly into the cell.

In the steady state,

$$\bar{x}_i = \alpha_{i,i}\,\bar{x}_i + \alpha_{i,i-1}\,\bar{x}_{i-1} + u_i,$$

and it follows that:

$$\bar{x}_i = \frac{\alpha_{i,i-1}}{(1-\alpha_{i,i})}\,\bar{x}_{i-1} + \frac{1}{(1-\alpha_{i,i})}\,u_i = \gamma_i\,\bar{x}_{i-1} + \delta_i\,u_i,$$

where $\gamma_i = \dfrac{\alpha_{i,i-1}}{(1-\alpha_{i,i})}$, $\delta_i = \dfrac{1}{(1-\alpha_{i,i})}$.

Knowing the steady-state solutions $\bar{X}_1$ and $\bar{X}_2$ for two different discharges U_1 and U_2, we may calculate the γ_i and δ_i, and hence the $\alpha_{i,i}$ and $\alpha_{i,i-1}$, and then may use the general equations (1), and (2) for further analysis of $\bar{X}$, U, and B.