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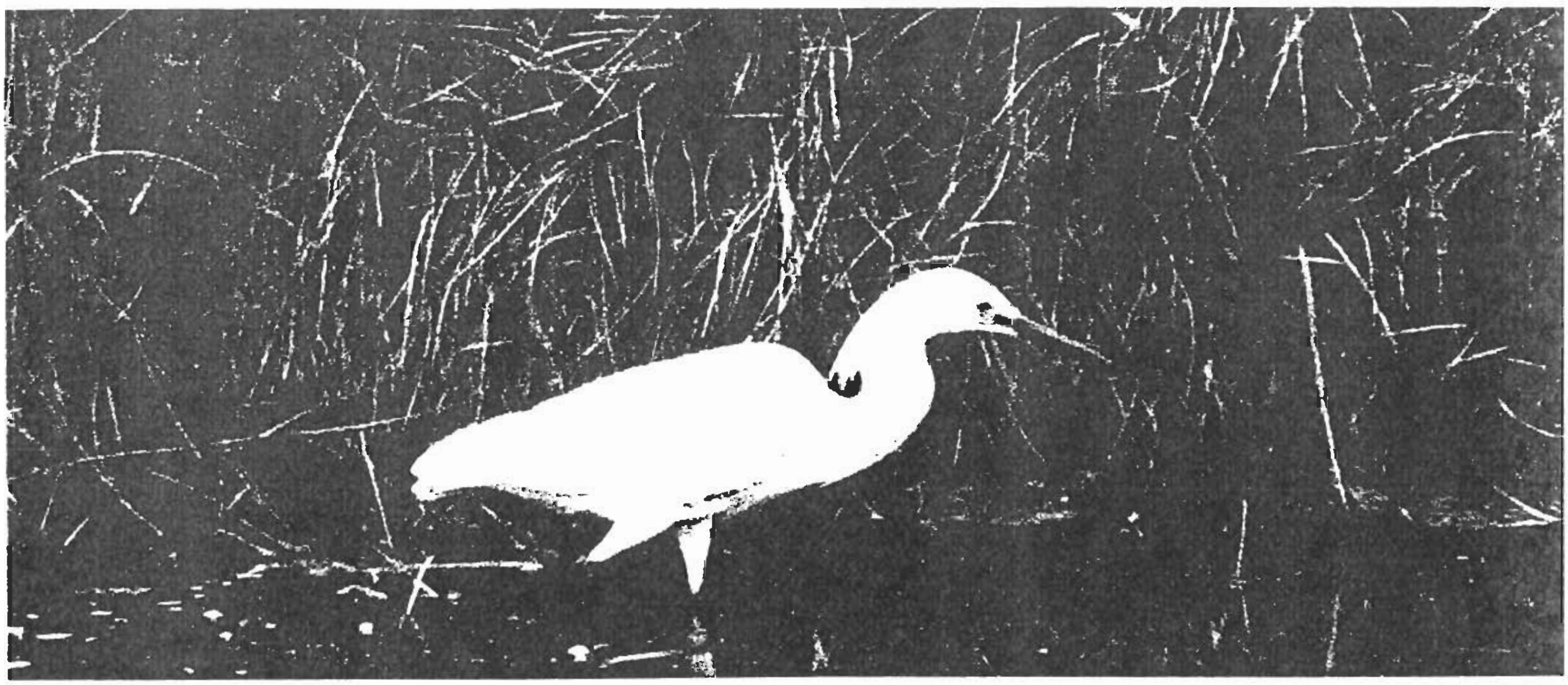
Appendix A: Strategies for Sources, Transport and Fate Research



Report of the Subcommittee on Sources, Transport and Fate

Research Strategies Committee

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U. S. Environmental Protection Agency
Science Advisory Board
Research Strategies Committee
Sources, Transport and Fate Subcommittee

Chair

Dr. George Hidy
Electric Power Research Institute, Environmental Division
3412 Hillview Avenue
Palo Alto, CA 94303

Members

Dr. Anders Andren
University of Wisconsin, Water Chemistry Laboratory
660 N. Park Street
Madison, Wisconsin 53706

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National Center for Atmospheric Research
1850 Table Mesa Drive
Boulder, Colorado 80303

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University of California at Los Angeles,
Chemical Engineering Department
Boelter Hall
Los Angeles, CA 90024

Dr. Richard Conway
Union Carbide Corporation, South Charleston Technical Center
3200 Kanawha Turnpike (Bldg. 770)
South Charleston, WV 25303

Dr. Robert Huggett
Virginia Institute of Marine Science,
School of Marine Sciences
9 Raymond Drive
Seaford, Virginia 23696

Dr. Donald O'Connor
Manhatton College,
Environmental Engineering and Science Program,
Riverdale, New York 10471

Dr. Barbara Walton
Oak Ridge National Laboratory, Environmental Sciences Division
Post Office Box X
Oak Ridge, TN 37831-6083

Dr. Herbert Ward
Rice University,
Department of Environmental Science and Engineering
6100 South Main
Houston, TX 77005

Support Staff

Dr. Donald G. Barnes*
Acting Staff Director, Science Advisory Board
U.S. Environmental Protection Agency

Ms. Joanna Foellmer
Secretary to the Staff Director, Science Advisory Board
U.S. Environmental Protection Agency

* Original draft prepared through the support of Dr. Terry F. Yosie, former Director, Science Advisory Board

Strategies for Sources, Transport and Fate Research

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STRATEGIES FOR SOURCES, TRANSPORT AND FATE RESEARCH

1.0 Executive Summary

Sources, transport and fate (STF) research explores the interconnections between sources of environmental pollutants, their transport and transformation through the environment, and their ultimate fate. These research findings allow measurement or prediction of pollutant concentrations at points distant from the source. These exposure data are coupled with toxicity information to assess risk. In other cases, STF research can be used to identify sources of environmental risks. For example, previously unsuspected pollution sources fortuitously have been identified through field measurements (e.g., chlorinated dibenzo-p-dioxins from pulp and paper mills), and mathematical models have successfully related suspect source emissions to particular environmental findings (e.g., stratospheric ozone depletion). In addition to risk assessment purposes, STF research is being looked to as a generator of "early warning" information on potential, emerging, and/or escalating environmental problems.

In order to meet these growing demands, STF research strategy in the 1990's should have two major elements, which are central to this report:

a. Strengthening EPA's capability for predicting environmental form and concentration of pollutants, with a known level of uncertainty, through measurements and modelling.
b. Utilizing STF knowledge to provide an early warning vehicle for anticipating issues that are likely to become priority concerns for EPA.

The first element of the strategy calls for expansion of the knowledge base on transport and transformation processes in order to develop and validate models needed in the assessment and management of environmental risks. The second element is designed to raise Agency and public awareness of environmental problems at a stage early enough to permit adoption of a cost-effective approach to risk reduction.

Regarding the first strategic element, much of the success of STF research depends upon the development and validation of mathematical models, specifying their degrees of uncertainty. While the basic principles applicable to many of these models are known, site-specific conditions, process data needs and differing scale requirements (e.g., local vs. regional vs. global, or short-term vs. long-term) limit the current successful application of these models and introduce uncertainties which need to be identified, quantified, and narrowed.

Models are predicated on mass conservation and, necessarily, require data on source characterization, media transport and chemical conversion processes, and deposition or media removal processes, which are sometimes called "fate" terms. A broad range of known and potential sources in all media (e.g., air, surface water, ground water, and soils) should be characterized through a core program examining the chemical characterization, release rates, and frequency of releases from the sources. This source information, coupled with fundamental knowledge of transport and transformation processes, should feed into the mathematical models which predict the behavior and ultimate fate of the pollutant(s) in various media and generate estimates of exposure.

Regarding the second major element of the strategy -- the need for early warning --, great benefits can be derived from early identification of problems; i.e., reasoned risk reduction actions can be implemented to correct a situation before it requires a costly crisis response. The ability to detect problems before they would traditionally appear is related to foresighted collection and judicious use of key environmental data. Chemical, biological and physical monitoring activities, a major source of such data, need to be strengthened considerably.

In addition, a shift in strategic thinking is needed in the basic approach to environmental monitoring. Currently, the Agency focuses on a limited number of selected pollutants, adopting a "feedback" strategy. That is, if certain pollutants are found in excess of some existing standard or limit, the information is fed back and regulatory action is taken. In the future, the Agency should adopt a "feed forward" strategy that involves monitoring a much broader range of compounds and other environmental stressors of potential interest, many of which do not have regulatory standards. The resulting data would provide an increasingly realistic and complete estimate of the total toxic burden in the environment and a context within which to determine more easily the extent to which chemically transformed products or new, unregulated compounds enter the environment. It would also highlight situations in which the distribution of chemicals change, perhaps indicating significant changes in environmental conditions; e.g., global air (climate) warming from the increased presence of radiation- absorbing gases in the atmosphere. Such information would be fed forward and analyzed, possibly leading to the development of a regulatory or other risk reduction response.

Careful consideration of societal, economic and technological trends could also be helpful in anticipating--and possibly avoiding--environmental problems. Measurements alone will not suffice to provide an anticipating framework. A forward looking analysis also will be needed. The Agency should assign the task of achieving this "early warning" goal to a group charged with discerning the implications of emerging observations and knowledge in the context of past knowledge. This group would submit an annual report on their findings and projections, or a special alert of findings as necessary.

This Report contains three specific recommendations:

a. Recommendation I: Improved STF Models
EPA should strengthen its research on STF model development, evaluation and validation, as a means for reducing uncertainty in risk assessment and risk management.

b. Recommendation II: Leadership by the Risk Assessment Council
The Agency's Risk Assessment Council should take steps to insure that STF research is integrated into EPA's approach to exposure assessment analyses.

c. Recommendation III: Establishment of Early Warning Group
The Agency should establish a group of senior scientists and engineers to identify potential, emerging, and/or escalating environment health and ecological problems using systematic, long term measurements and their interpretation.

2.0 Importance of Source, Transport and Fate Research

2.1 The Role of Sources, Transport and Fate Research

The study of the sources, transport and fate (STF) of pollutants is an essential part of environmental research. This type of work has served three major roles in environmental assessment, resulting in the ability to estimate exposure concentration levels and to relate excessive exposure levels to sources needing emission reduction. The roles are:

a. Generation of fundamental knowledge about the physical and chemical characteristics of emissions from pollution sources.
b. Clarification of the nature of transport, conversion and media loss processes (e.g. deposition and absorption) that lead to exposure.
c. Highlighting of chemical conversions leading to pollutants that differ from the direct emissions; e.g., the conversion of sulfur dioxide into sulfuric acid in the atmosphere.

In the first instance, an expanding inventory of compounds or radioactive substances has emerged that potentially affect the environment. In some research the interpretation of temporal and spatial distributions of ambient measurements has led to the identification of sources otherwise not considered (e.g., polychlorinated dibenzo-p-dioxins from pulp and paper mills). Accurate source identification information is important for the development of cost-effective control strategies.

Second, STF research has provided the principal basis for developing mathematical models to relate source emissions to ambient conditions, yielding exposure estimates. Such models provide a critical element of exposure estimation in space and time to assess the impact of both existing and new sources. Particularly notable accomplishments of modeling that have not only provided regulatory tools but have advanced the understanding of source-receptor relationships include multiple source air dispersion models and chemical fate models for ground water contamination.

Specially designed measurement programs have been required to provide data to investigate environmental processes and to verify and test the reliability of such models. These measurements are distinct from monitoring and surveillance for existing regulatory requirements.

A third role of STF research involves understanding large-scale environmental phenomena, using basic knowledge of chemical processes, results from laboratory experimentation, development of mathematical models, and critical measurements in the field. Examples of major contributions in this category include:

a. Tropospheric ozone prediction schemes employing meteorological factors and highly complicated chemistry.
b. An explanation of the role of chlorofluorocarbons in modifying stratospheric ozone,
c. The discovery of organic chlorine compounds in treated drinking water.
d. The exploration of complex bio-geochemical factors affecting the speciation of heavy metals such as mercury, chromium and selenium.

An additional emerging role of transport and fate research concerns the identification, analysis and interpretation of certain long-term trends that can alert policy makers to significant environmental issues in the future. Those have included inferences from long-term monitoring that emerged through ecological and biological effects, acid deposition and long-range transport, the build-up of greenhouse gases to produce climate change, surface hydrogeological concerns in the storage and land disposal of wastes, and identification of global contamination of the oceans from certain pesticides.

The past successes of STF research in raising scientific and public awareness on a wide range of environmental issues indicates that the public investment in this work is well founded. The area should continue to be an important component of EPA efforts in research and development.

2.2 Key Elements Needed in Sources, Transport and Fate Research

An important factor in risk assessment is knowledge of the sources of pollutants and the processes that subsequently govern the dispersal of a pollutant into the environment. This relationship can be conceived as links in a chain beginning with pollutant emissions followed by transport, transformation and media removal (deposition or sorption). Understanding these relationships contributes scientific insight as to how pollutants, through space and time, reach humans and other receptors. In addition, definition of source-receptor relationships aids decisionmakers in targeting specific sources for risk reduction efforts. Failure to address these questions can result in environmental policies and regulations that are cost-inefficient, spending too little on some problems and too much on others.

EPA's research has contained a substantial component of STF work in the past. However, the effort frequently has been poorly defined and, consequently, has not always focused on issues central to the Agency's needs. For the 1990's, STF research strategy should have two major elements:

a. Strengthening the capability of predicting environmental form and concentration of pollutants, with a known level of uncertainty, through measurements and modeling.

b. Utilizing STF knowledge to provide an early warning vehicle for anticipating issues that are likely to become priority concerns for EPA.

The first strategic element would expand the base of knowledge on transport and transformation processes in order to develop and validate mathematical models for assessing and managing environmental risks through exposure estimation and identification of significant sources and their relative contributions. The second goal would use a combination of measurements, theory and analysis to contribute to raising Agency and public awareness of issues potentially harmful to public health and the environment at a stage early enough to permit adoption of a cost-effective approach to risk reduction.

Section 3 discusses these key elements of the STF research strategy. Section 4 offers specific recommendations.

3.0 Strategy for Sources, Transport and Fate Research

Environmental risk assessment and management requires reliable means for estimating exposure in space and time, as well as estimating the contribution of sources to those exposure patterns. Exposure to humans and to ecosystems can occur through respiration, ingestion, direct contact, or the food chain. Exposure generally is defined in terms of an ambient concentration or bioaccumulation concentration over time, a deposition rate to a collector, or a total medium burden (amount of material in a defined volume). In the absence of direct measurements of exposure, estimation of concentration, deposition or burden can be carried out through interpolation or extrapolation of results of mathematical calculations based on the principles of mass and energy conservation. Continuing research is needed on both direct measurement of exposure and predictive models, as discussed in the report of the Exposure Assessment Subcommittee. In general, projections of source contributions to exposure at a receptor (source-receptor relationships, or SRRs) presently can be done only through mathematical models.

Inherent in either the interpretation of field observations or mathematical modeling are uncertainties in exposure or SRRs that are seldom known. A scientifically supportable risk assessment requires an accurate and precise exposure estimate. Therefore, determination of uncertainty in estimates is as important as the estimate itself. This is also true in risk management where a balancing among cost, technological effectiveness and reliability, and other factors is often required or used for selecting among determining emission control options. Inherent in the improvement of risk methodology is reduction of uncertainty in estimates of the attribution of exposure to specific sources.

Uncertainty in exposure estimation derives from two factors. The first concerns a mismatch in the spatial or temporal scale of calculations relative to receptors. The second uncertainty stems from errors in the models themselves, the input data to the models, and computational errors inherent in numerical techniques which are employed in the execution of the model.

Models calculate concentrations or burdens in a relatively coarse or macro-scale. An individual receptor generally is much smaller than this resolution and often is mobile. These factors make it necessary to use population mobility and statistical factors to relate measurements at fixed stations and model calculations to receptor exposure. Little research has been done to reduce uncertainty in these factors or in estimation of target tissue doses resulting from environmental exposure. This subject is more fully discussed in the report of the Exposure Assessment Subcommittee.

Work has been done to define uncertainties in model calculations but, in general, models and interpolation schemes are not well tested for reliability or validated for the quality of their simulations.

The validation of theoretically based models is often defined at two performance levels. The first is determined by a suitable comparison of its predictions with ambient concentration measurements for given physical or chemical input conditions. However, close correspondence between model prediction and a few, selected environmental measurements does not necessarily constitute adequate model validation. Thus, a second validation criterion is needed that tests the model for its integrity in simulating media processes that link source emissions to ambient conditions. Testing models at this level is far more demanding than the first evaluation, but it needs to be an integral part of STF research. Experimentation with models at this level leads to advances in basic knowledge as well as added confidence in the model performance.

3.1 FIRST STRATEGIC ELEMENT: Reduction of Uncertainty in Estimating Environmental Concentrations of Pollutants.

3.1.1 Modeling and Model Validation

Effective risk assessment begins with an attempt to estimate the environmental concentration of contaminants within an acceptable margin of error, followed by exposure assessment that assumes a reasonable level of confidence in estimates of contact with these environmental pollutant concentrations. Three factors significantly affect the accuracy of estimates of environmental concentration:

a. Specification of source location, chemical characteristics and emission rates.
b. Description of transport and chemical conversion processes.
c. Description of fate or removal processes.

Information on these factors is used to construct models to represent the phenomena believed to be involved in the movement and transformation of chemicals in the environment, and computer codes are developed to facilitate what are frequently very complex calculations.

The EPA requires reliable data on concentrations in environmental media in order to determine exposures to target organisms and populations for risk assessment. The Agency also requires data on the contribution of specific sources to pollutant concentrations (i.e., SRRs) as a means of identifying which sources to target for reducing risk. In the absence of sufficient data on exposures, source data may be combined with transport and transformation models to provide estimates of exposure. In such cases, it is critical that the models be capable of providing exposure estimates within acceptable (or at least defined) bounds of uncertainty. Uncertainty is determined by the suitability of the model (i.e., whether it includes appropriate terms for all of the important variables, such as dispersion and meteorological conditions) and by the accuracy of coefficients and other input data associated with each variable or connecting mathematical term. In an ideal world, each model would be fully validated before it is used for risk assessment or risk management decisions. However, the high costs and long lead times required for model validation inhibit the validation effort in a regulatory agency such as EPA.

In reality, a model can prove useful, even without a full validation, provided that it can be empirically verified for a range of conditions comparable to those in the situation for which it is to be applied. Furthermore, as it is applied more widely and tested periodically against available environmental data, it can be refined and/or modified, based on operating experience. Thus, iterative applications of models have served the EPA in several ways. They help to define the bounds of uncertainty associated with use of the model in risk assessment or risk management, thereby increasing confidence in the results. At the same time, the data generated provide a basis for refining the model and/or extending the bounds over which it can be used.

Although STF models primarily have been structured to address a single medium of the environment--air, surface water, ground water or soil--, it is increasingly apparent that intermedia and multi-media models are also necessary to analyze certain problems. In any case, the most general and appropriate structure of a model is based on the conservation of mass or continuity principles, incorporating source, transport, transfer and transformation components.

The basic principles that underlie any modeling effort are at least qualitatively understood and the numerical coefficients relating to the above mentioned components often can be estimated. The application to a particular problem, however, often requires more detailed qualitative descriptions of transport and transformation processes; e.g., resuspension of aerosols from soils and the role of wet scavenging of reactive organics. In addition, more accurate quantitative measures of the coefficients which model these processes may be required in order to obtain projected estimates that are of practical use to the risk manager. Thus, there arises the need for model calibration and validation specific to the problem and region, the degree and extent of which should be guided by the significance of the question and the environmental and economic consequences. EPA should continue to establish a systematic procedure and a specific schedule to validate key environmental models. This effort should include documenting underlying assumptions, updated modeling procedures and protocols, and estimating uncertainties in prediction capability for a range of conditions.

The verification of models to a defined uncertainty requires a combination of special data acquisition, including source emission and field tests, laboratory experiments, and theoretical or mechanistic studies of media processes. These generally involve progressive and incremental design considerations based on a continuing improvement in our knowledge.

The model components to be quantified are source characterization, media transport and conversion processes, and ultimate disposition ("fate") processes. Each of these components and their associated uncertainties are discussed in the following sections.

3.1.2. Source Characterization

In deriving estimates of environmental concentrations of pollutants, quantification of sources, their strengths, and interactions is potentially one of the larger sources of uncertainty. Because of legislative mandates, source inventory and characterization have been directed toward release into specific environmental media such as air, surface water, ground water and soil. Great strides have been made on emissions estimation in the last 15 years; however, source characterization should continue to be high in priority because

a. Historical sources such as abandoned waste pits and dumps have been inadequately characterized as to the presence of particular pollutants or to releases.
b. More recently acknowledged sources, such as contaminated sediments, present additional assessment problems
c. Advances in emission control technology and evolution of industrial processes and activities require progressive re-evaluation of emissions inventories
d. Multi-source and multi-media interactions have been inadequately characterized.

The sources to be studied will change according to the prioritization of current and projected environmental problems and introduction of new technology. Within a given problem area, the sources studied should not be limited to those addressed by current Federal regulations. Rather, the outlook should be as comprehensive as possible to define the magnitude of current and emerging problems. In studying ground water pollution sources, for example, municipal landfills should be included as well as RCRA Subtitle D facilities and the use of agricultural chemicals. Source research should address area, as well as point, sources and both mobile and stationary sources. A continuing core research program in this area is recommended both to develop generic methodology and to apply it to critical environmental problems. Three aspects of a core program are addressed in this report: chemical characterization, release rates, and episodic releases. Emphasis also should be placed on emerging technologies and new chemicals entering the environment.

3.1.2.1 Chemical Characterization

The objective of chemical characterization is to develop and apply efficient methods that adequately define problem sources and point to solutions. Accuracy, precision, detection limits, matrix effects, cost, and time are all critical factors. Besides the identity and concentration of chemical constituents, tests are needed to predict the mobility of materials under various scenarios and to provide data for selection/design of control techniques.

3.1.2.2 Release Rates

Emissions from point sources often can be directly measured, while the flux of contaminants from various area or diffuse sources into the environment is estimated by applying a mathematical model to either source characterization data or ambient monitoring data. Each approach is associated with levels of uncertainty that need to be established and then reduced when greater accuracy and precision is required. For example, many exposure estimates assume a nominally steady discharge of a pollutant, when in fact, variation in emissions rate may be critical to an accurate estimate of exposure. Also, there is a need to develop approaches which utilize all available data sources, be they NPDES reports, air permits or RCRA Part B applications. Improved release rate models need to be soundly conceived and adequately verified for a variety of applications.

3.1.2.3 Episodic Releases

In many situations EPA may emphasize the regulation of emissions under stable, steady conditions while serious environmental and/or human health problems are caused by sudden releases or "upset" conditions. Formal procedures are needed for:

a. Identifying specific potential hazards; i.e. situations that could result in a sudden release.
b. Estimating probability of that hazard occurring.
c. Predicting the magnitude and chemical or physical form of the release.

Projections of equipment failure and handling or transportation accident rates are needed. Acceptable standards of practice need to be established and tested. One approach for hazard identification is to divide operations into segments and compare possible risks against a hazard checklist, including combustible mixtures, mechanical stress, vapor cloud release and over-pressurization. The potential for natural disasters, like a sudden gas release (e.g. carbon dioxide or hydrogen sulfide) from a volcanic disturbance or a deep lake sediment should be investigated.

3.1.2.4 Source Characterization by Medium

3.1.2.4.1 Air

Although air quality research is said to be more advanced than research for other media, a continuing effort will be needed to refine and improve knowledge of emissions for regulatory decision making. Over the past decade there has been considerable effort to characterize emissions of criteria pollutants and certain hazardous chemicals from stationary and mobile sources.

Data acquisition for source characterization will be needed for air regulatory analysis at a modest level of priority for at least the next decade. Continuing work will be required to maintain and update the inventories. Characterization of emissions from new or rebuilt facilities will be required, as will the estimation of pollutant forms not previously considered.

Additional research will continue to be needed to provide improved emission factors and to define the uncertainties and limitations in available data. With such refinements, high priority should be assigned to upgrading estimates of emissions of nitrogen oxides and volatile organic compound emissions for use in source-receptor modeling and control strategy analysis of oxidants and air toxics.

3.1.2.4.2 Surface Water

In many instances non-point sources are the major contributors to freshwater surface problems; e.g., toxics in Lake Superior and Lake Michigan. Risk reduction efforts will increasingly turn to non-point sources because of the large fraction of surface water pollution problems they may represent and since point sources have been more effectively controlled.

Potentially important non-point surface water pollution sources include the following: run-off and leachates from agricultural and other land uses, deposition of wind-borne volatile organic chemicals and heavy metals, groundwater inflow and sediment releases. At this time source models for predicting organic loadings are much further developed than models for inorganic loadings. Also, agricultural run-off is considered to be better characterized than is urban run-off. Research should be balanced between monitoring (direct measurements for use in identifying/defining problems, as input data to models, and in model validation) and development of predictive run-off models. Specific models need couple the source information with hydrodynamic and process kinetic models, describing sediment transport, and elucidating biologically mediated reactions, metal speciation kinetics, and hydrophobic compound transport. Reconstructive models based on concentrations in receptor organisms, including humans, also are useful. Balanced funding of field measurements and predictive modeling is recommended.

3.1.2.4.3 Ground Water

Contamination of ground water from human activities frequently originates from surface impoundments, landfills, agriculture, leaks and spills, septic tanks, mining, petroleum and gas production, and underground injection of wastes. EPA's 1977 "Report to Congress on Waste Disposal Practices and Their Effects on Ground Water" (Premier Press, Berkley, CA, 1980) identified the disposal of wastes at industrial impoundments and other solid waste disposal sites as the most important sources of groundwater contamination. It estimated that approximately 15% of the liquid and solid industrial wastes generated in the United States can be classified as hazardous. Such wastes represent potential sources of groundwater contamination, depending on the method of disposal. Most of the past land-disposed wastes were not managed by means that comply with more recent Federal regulations, and, therefore, they may threaten groundwater quality in many areas.

In addition to industrial wastes, the 1977 report identified so-called secondary sources of national importance including septic tanks, municipal wastewater, mining, and petroleum exploration and production residues. Although concentrations of toxic material from these sources are generally lower than from industrial wastes, they can be significant on a regional basis. In an area of substantial manufacturing activity containing large numbers of people, there exists a potential for pollution of groundwater resources, especially from products such as gasoline, fuel oils, and solvents. Areas where mining, agriculture, and/or petroleum production are prevalent are also at potential risk.

3.1.2.4.4 Soils and Sediments

Soils and sediments can retain organic and inorganic chemicals released to the environment. Therefore, they can become sources for release and subsequent contamination of air, ground water, and surface waters through resuspension, vapor losses, leaching, and removal of particulates containing sorbed compounds. Defensible risk assessments and risk management strategies require reliable information on the amount of contaminants accumulated in soils at sites and knowledge of how to predict contaminant persistence, transformation, and transport to other media.

The spatial distribution of chemical contaminants in soils is often extremely heterogeneous. Consequently, extensive core sampling and/or exhumation to delineate zones of contamination can be time-consuming and expensive. In situ and remote assay equipment and sampling methods are needed to determine concentrations of chemicals in surface and subsurface soils. Among approaches that show promise are those that couple recent advances in laser technology with those in fiber optics in order to improve the detection of organics and the development of portable gas chromatographs for analysis of volatile organics in the field. In addition, neutron and scintillation probes may prove useful for in situ detection of transuranic and gamma-emitting radionuclides, respectively. Development of these and other techniques to detect and quantify contaminants will require a significant research effort, but one that would yield a high payoff in monitoring capability.

In order to adequately assess soil sources, there is a need for appropriate leaching test(s). Improved methods are needed to evaluate contaminated soils and wastes to account for variability in leach rates of constituent chemicals over a long period of time at specific sites. Such methods could be used to improve cleanup and closure of RCRA and CERCLA sites, as well as to serve as guidance for management of land treatment and landfill facilities.

3.1.3 Transport Processes

There is general acceptance of the basic principles of the transport component of STF models. The fundamental equations of fluid (air and water) motion which follow from these principles are reasonably well-established and have been utilized for calculations. The principal limitations of these models often lie with certain empirical transfer coefficients that are media specific. The mixing and dispersion associated with the fluid motion, although understood, has less of a research base to support it. Nevertheless, empirical relations, based on field and laboratory data, provide important insight into the nature of transfer coefficient variability. The recent advances in turbulence theory increase scientific understanding of this important mixing mechanism. At the present time, the development and application of fluid dynamic models incorporating this theory reside primarily with the research scientists. Transferring this knowledge to the environmental analyst is an important need for the future development and application of air and water quality models. Certain specialized areas; e.g., underlying sediment bed failure, remain as more fundamental challenges for environmental modellers.

Analytical and numerical solutions and the associated codes are available for surface and ground water transport models. Stochastic or Monte Carlo techniques have also been used to define the uncertainty of the various elements in these models. Different research groups should test a selected group of models in order to determine those which are most appropriate for use in environmental quality analysis. This testing should be followed by a comparison of model performance with sets of observations from various air regimes and water systems.

3.1.3.1 Surface Water

The transport of pollutants in freshwater bodies is predominantly advective (moving with the mean flow), rather than dispersive (associated with the eddying). Given the knowledge of the hydrologic balance of a drainage area and empirical correlation of the dispersion, transport of pollution in freshwater systems can usually be determined with greater accuracy than some other components of the mass balance; i.e. sources and transformations. The hydraulic interaction (e.g., caused by fluctuating levels) between the surface and ground water deserves further attention as it relates to estimating contamination.

The dispersive component in estuarine and coastal systems is more significant than in fresh waters. In the former, the effects of density stratification on vertical and lateral dispersion and the distribution and disposition of sediment and organic particulates needs to be further developed. Given the intensive computational manipulations required to solve multi-dimensional fluid dynamic/quality models, a significant effort is needed to enable these models to interact for long-term, time variable simulations and projections. Much remains to be done on transitions for coastal systems both on the east and west coast of the country. The eddies from the Gulf Stream in the Atlantic have marked effects on the transport within the region north of Cape Hatteras and notably in the New York Bight. The Gulf Stream has not been successfully modeled in spite of the advanced state of knowledge of the field and aforementioned developments.

Wind and temperature effects are important factors in defining transport in marine systems, as well as in lakes and reservoirs. The latter have frequently been modelled in a simplistic fashion by assuming complete mixing. For long term projections this approximation has been successfully applied in many cases. For the more refined, multi-dimensional analysis, however, much needs to be done in applying turbulence theory to the analysis of transport phenomena in lakes and reservoirs so that detailed concentration patterns can be estimated. In addition, intermedia transfer phenomena (e.g.,the role of the surface microlayer in pollutant transport across the water/atmosphere interface and critical factors in water/sediment transfer) need additional study.

3.1.3.2 Ground Water

As in the case of surface water, the basic equations of fluid motion in the saturated zone of ground waters are generally well established and understood. Qualitatively, fluid transport in some important ground water media has successfully been modeled. Similarly, the dispersive effects, referred to as dispersivity, have been empirically defined to some degree, but site-specific evaluation of this component is usually required. By contrast, knowledge of the transport in the unsaturated zone is inadequate, and further development in this area is needed. A major source of uncertainty in groundwater modelling is the inherent heterogeneity of the soil media and underlying rock structure, which must be addressed on a site-specific basis.

3.1.3.3 Water-Underlying Bed Interactions

The exchange between the water and the underlying sediment bed acts as both source and sink of dissolved and particulate forms of pollutant constituents. In some cases, the transfer rates from or to the bed far exceed the current mass inputs from point and non-point sources. Two general constituent categories are considered: nutrients and toxic substances. The former affects the bacterial and algal levels in the water column. In many locations this interaction is the major factor in a dissolved oxygen budget. There is a pressing need for the analysis of dissolved oxygen and eutrophication to better characterize the flux of nutrients at the water-underlying bed interface.

Many organic chemicals and heavy metals partition to particulate matter, particularly to the organic and clay fraction of the solids. The degree to which the contaminated particulates accumulate in the sediment depends on the characteristics of the solids and the turbulence and shear at the water-underlying bed interface. Estuaries, lakes or reservoirs are net sedimenting systems and accumulate these toxic substances in the bed. The broad area of sediment interaction with the water column in all systems requires a significant effort in order to understand the phenomena of sediment transport, settling, resuspension and bioturbation affecting water quality.

3.1.3.4 Soils

Current methods are inadequate to predict accurately conditions in soils (e.g., moisture and temperature fluctuations) or the transport of organic and inorganic contaminants in this medium. Studies are needed to refine the conceptual models for organic and inorganic mobility and to provide for the influence of soil heterogeneity and other environmental variables on these processes. Structure-activity analyses should be explored to improve predictions based on physicochemical properties of specific compounds.

Pollutant transport through soils is often viewed simply as a single chemical chromatographic process. This view fails to account for the influence of soil structure (e.g., macropores), rainfall events, contaminant interactions in waste mixtures, and the possibility of movement via colloidal transport and adsorption to mobile microparticulates. Studies are needed to delineate the extent to which these additional processes affect rates of contaminant transport in soils.

3.1.4 Fate Processes

The environmental fate of a substance depends on physical dispersion processes as well as on its physical, chemical, and biological properties or interactions with substrates. Information required for future predictions of the fate of chemicals in air, soil, or water includes such basic data as aqueous solubility, vapor pressure, air-water partition coefficient (Henry's Law constant), molecular diffusivity, phase partition coefficient, melting point and absorbtivity. There has been progress in acquiring data in pure homogeneous systems. This fundamental information is needed in order to understand the effects of cosolvents, unicelles, and colloids on these properties. In addition, many chemicals hydrolyze, photolyze or participate in additional abiotic or biotic degradation processes, such as electron transfer reactions. An increased effort is needed to produce thermodynamic and kinetic data for heterogeneous systems as well; e.g., the influence of metal oxides and microorganisms on the persistence of chemicals in soils.

Since economic and logistical constraints prohibit laboratory measurements for all these properties and rate constants, an alternative predictive tool is recommended: investigation of chemical structure-activity relationships. These estimated parameters are then adapted for appropriate fate models. Such an approach has been used with great success in chemical engineering to design unit processes for chemical manufacturing and in pharmacology to construct pharmacokinetic drug transport models.

3.2 SECOND STRATEGIC ELEMENT: Early Detection of Environmental Problems

3.2.1 New Stressor Identification: The Need for Early Warning

Early identification of potential, emerging and/or escalating environmental problems should take its place along with risk assessment and risk management as a central part of EPA's mission. The current research program provides no funds specifically earmarked toward this objective. This is disappointing in view of the number of issues (e.g., radon, stratospheric ozone depletion and global climate change) that have only recently risen to priority in EPA's policy agenda but which have been known to the scientific community for a number of years. It is also surprising because of relatively high perceived risks and the rising priority for these "newer" problems which are discussed in EPA's February, 1987 report entitled "Unfinished Business: A Comparative Assessment of Environmental Problems" (EPA/230/2-87/025a-e). While admittedly not a scientific study, the "Unfinished Business" report provides a rationale for follow-up investigations that need to be pursued, if only to minimize future surprises and to ensure a better match between research expenditures and significant sources of public health and environmental risk.

The benefits of early identification of stressors to human health and ecological systems include:

a. Cost reduction: more orderly conduct of the research vs. expensive crash programs.
b. Improved regulation: more time is available to develop data bases for scientifically supportable regulations.
c. Risk reduction: steps can be taken early to reduce or prevent risk either by non-regulatory and/or regulatory means.

Initiation of a program to identify new or potential risks, which can complement the Agency's ongoing efforts to assess known risks, is strongly recommended.

3.2.2 Early Warning Data Sources

3.2.2.1 Chemical, Biological, and Physical Monitoring

Many of the environmental stresses that concern this nation and the world are caused by anthropogenic chemicals. Often a crisis is first detected through the direct observation of a biological effect caused by pollutants rather than by earlier prediction or detection of the release. There are numerous examples of this pattern, including:

a. Kepone in the James River detected by the observation of worker illness.
b. Tributyltin in harbors detected by the observation of malformed oysters.
c. Polybrominated biphenyls in Michigan cattle detected by the observation of dead and dying animals.
d. Polynuclear aromatic hydrocarbons in areas of the Puget Sound detected by the observation of fish with cancers.

Often by the time a problem is detected, biological damage has already occurred and remediation is difficult, expensive or impossible from a practical standpoint. In other words, the anticipatory regulatory systems have been inadequate.

Improved anticipation can be promoted through an improved surveillance system. Such a system would continue to include a chemical monitoring program designed to quantify a preselected set of compounds already of regulatory interest. This approach has been the thrust of most environmental monitoring to date. An improved surveillance system should, in addition, provide qualitative identification of additional chemicals of concern. This latter approach has been haphazard in deployment, but has proven important.

There are advantages and disadvantages to the first, directed approach. One advantage is that the qualitative aspects of chemical analyses are simplified. Analytical methodologies can be selected or developed for specific compounds, decreasing the possibility of false identification. The quantitative outputs of the analyses are usually more accurate and precise because the methodologies employed are optimized for the preselected compounds. These outputs are particularly important if the objective of monitoring is to determine compliance with some regulatory program or permit.

A disadvantage of the directed approach is that only the preselected compounds are surveyed even though other compounds may also be detected. The data for the latter compounds are generally ignored and even lost. New compounds, which may later prove to be damaging to human health or the environment, are not systematically tracked. Examples exist where chemical problems have been needlessly overlooked. Among these are the impacts of such organic chemicals as polychlorinated biphenyls in the 1960's, Kepone and dioxins in the 1970's. In other words, potentially valuable chemical data have not and are not being utilized specifically for environmental assessment because of a narrow focus on chemical-specific monitoring.

Another way of describing most existing monitoring systems for toxic chemicals is to describe them as "feedback" programs. Such feedback programs are keyed by error signals. For example, if a permit allows a certain amount of a specific compound in an effluent, a concentration that exceeds the permitted level by an established margin constitutes an exceedance; i.e., a violation. Detection of this violation may feedback, initiating regulatory action. Compounds not specified in a permit and, therefore, not analytically sought, cannot trigger an warning alert even though these "new" compounds may be detrimental to the biological communities in the receiving media. —

Technologies and expertise now exist to reduce such oversight through improved design of broad-based chemical monitoring programs and the use of biological endpoints in monitoring. The use of techniques such as gas chromatography (GC) and gas chromatography-mass spectrometry (GC-MS) provide effective means for efficient, anticipatory monitoring. Through the use of various columns and detectors, these methods yield signals for essentially all of the compounds present, both those which are analytical targets and those which are unexpected. Even though many of the output signals are not essential to a feedback system, they can be collected, stored, and analyzed through the use of data handling systems. This broad-based record can be examined historically for chemicals of possible concern and for apparent shifts or trends that may signal an accumulation of material.

In such a program, data systems could be linked together to create networks. Software could be developed to query the networks to determine whether new chemicals have appeared between samplings and whether a compound is increasing or decreasing over time. The network could provide efficient access to the areal distribution of a compound(s) of potential interest.

This alternative to targeted chemical monitoring would sacrifice some quantitative aspects of the analyses in order to maximize the qualitative outputs. That is, this added information would be obtained at the cost of somewhat higher limits of detection.

The results of these refinements to chemical monitoring would be progress toward "feed forward", rather than feedback, monitoring. Feed forward monitoring, in this case, is defined as monitoring designed to determine when new, unregulated or unselected compounds enter a system and when shifts in the distribution of chemicals in the environment occur. Feed forward monitoring has the advantage of determining many more compounds, which in turn provides a much more realistic estimate of the total toxic burden to which organisms are exposed. Such information would be "fed forward" and analyzed, possibly leading to the development of a regulatory or other risk reduction response.

Although feed forward monitoring programs may be less cost-effective in the short-term than routine feedback monitoring for regulatory compliance, the long-term benefits of avoiding a future kepone-type event justify the costs associated with the development and maintenance of such an early warning system. Further, judicious application of knowledge about what biological and physical processes are possible can increase the efficiency with which feed forward monitoring is conducted.

Plants and animals can also be used to gain important information about the sources and availability to biota of chemical contaminants and their resulting effects. Insight can result from analyses of tissue that may not be possible from chemical analyses of abiotic components of ecosystems. Another advantage of biological monitoring is the extremely high sensitivity of certain biochemical endpoints, such as enzyme induction, that can supply evidence of the presence of chemicals at concentrations below thresholds for chemical analyses. Recently published studies have shown that biomedical tests derived from research on mammals are useful when applied to aquatic systems. The detection of chemical stresses on aquatic biota by utilizing histopathological and immunological techniques is now possible. The observation of tumors in fish from Puget Sound, the finding of lesions and depressed immune systems in fish from the Elizabeth River, Virginia, and the determination of elevations in metallothionein concentrations in fish from Prickley Pear Creek, Montana, are examples of the use of such technologies. Also, non-specific indicators of toxicant exposure can be valuable monitoring tools in broad-scale screening programs. For example, deviations from normal ratios of single-stranded to double-stranded DNA reflect exposure to a broad array of genotoxic chemicals.

There is no doubt that the ability to analyze environmental samples will improve and become more comprehensive in the future. There is also no doubt that the need for long-term monitoring data will increase as technology and human populations expand. Both of these developments support the concept of collecting and storing environmental samples to be analyzed in the future as new techniques become available or other needs dictate. The Agency now participates in such a program, the Environmental Specimen Bank. Consideration should be given to expanding the effort. The availability of documented samples on which to perform retrospective analyses could be extremely advantageous for determining temporal or spatial trends. Similar efforts should continue with the National Human Adipose Tissue Survey (NHATS).

Monitoring efforts should also address risks caused by stresses on humans and ecological systems other than direct toxicity of anthropogenic chemicals. These stresses include global warming, increased UV-B radiation, physical modification of habitat, radon, pathogenic and engineered organisms, and natural chemical emissions.

3.2.2.2 Societal, Economic and Technological Changes

Clues as to potential and emerging public health or ecological stressors (risk) can be gained by periodically examining societal, economic and technological trends. For example, energy conservation scenarios developed in the 1970's because of rising energy prices could have predicted the rising importance of indoor air pollution problems heightened by increasing insulation and resulting decreased ventilation. Similarly, more recent estimates that approximately 70% of the American people will live within 50 miles of a coastal area by the year 2000 strengthen the urgency for protecting estuarine and marine ecosystems. Other examples of trends which can be studied are the significance of superconductors, climate change and urban population changes.

Some aspects of such an effort were included in a 1980 ORD report entitled "Environmental Outlook 1980" (EPA-600/8-80-0003, July 1980). Potentially useful procedures of identifying the environmental impact of trends in energy supply/demand, demographics, human activities, economics, regulations, natural cycles, international activities, and technology are described. However, the thrust of the report was not on identification of new risks or rapidly escalating risks; rather, the report was directed at determining the effects of such trends on existing efforts to assess and control known risks. In order to make this risk-identification effort successful at a reasonable cost, greater emphasis needs to be on the identification of new, emerging, and rapidly escalating stressors/risks.

3.2.2.3 Literature Reviews and Expert Workshops

Selected literature should be monitored with the aim of searching for signals of new stressors. Also, workshops should be held at least annually to solicit the thinking of outside experts on potentially significant environmental problems. Possible mechanisms include utilizing units of the National Academy of Sciences, the National Academy of Engineering, the Office of Technology Assessment, professional societies or other Federal agencies to host or co-sponsor such workshops. Working with EPA, these and other institutions; e.g., NIEHS, can organize leading scientists, engineers, sociologists, economists, and others to identify potential and emerging ecological and health stresses.

3.3 Implementation by EPA

Essential to the development and success of an early warning system is the formation of a group of people within EPA that includes, at a minimum, staff drawn from the Office of Research and Development and the Office of Policy, Planning and Evaluation. The group would prepare analyses and studies of potential problems, draw upon other Agency expertise, as appropriate, and fund certain outside studies in the data source areas cited above. These people should be experienced individuals who can discern the implications of existing and new information and be able to assess its importance. Inclusion of visiting scientists from academia, industry or private groups would assist this effort by adding external inputs to the Agency.

Each year this group would prepare an annual report to the Administrator, Deputy Administrator and Assistant Administrators of new, emerging, and/or escalating health and environmental problems. The Assistant Administrator for ORD would develop a mechanism to ensure that the conclusions and recommendations of this group receive formal consideration in the research planning process.

4.0 Recommendations

4.1 Recommendation I: Emphasis on STF Models

EPA should maintain its research on sources, transport and fate (STF) model development, evaluation and validation, and continue improving its methods for reducing uncertainty in risk assessment.

To implement this recommendation, EPA should take the following actions:

a. Continue to formalize the mechanism and criteria for acceptability of STF models for all media, using methods such as the current procedures of the Office of Air Quality Planning and Standards (OAQPS).

b. Evaluate and validate on a priority schedule widely used STF models (single medium or multi-media), using a combination of field measurements and laboratory data to determine the level of uncertainties predicted by the models and to provide guidelines for reducing these uncertainties.

c. Continue research on media processes to ensure the quality of model input data in order to improve the detection and prediction of chemical transport and transformation in environmental media.

d. Adopt a systematic review schedule for STF model progress, including target milestones to achieve reduction in predicting uncertainties.

These four actions will facilitate the preparation of an orderly and focused Agencywide effort to advance the development and use of STF models in risk analysis.

Currently there exists a profusion of numerical codes that are exposure estimators. However, in general, they are not validated or tested, nor have they been ascribed specific quantitative uncertainties. The methods adopted by OAQPS serve as a useful Agency guide for placing a more uniform certification process on these types of models for regulatory analysis. Validated models are essential for this use so that public confidence in the reliability of risk assessment results can be increased. To achieve the goal of systematic and continued improvement of STF models, research funds should be provided to improve model input data for source emissions, fluid flow estimation, and physicochemical rate parameters. Improvements in these components need to be assimilated progressively into models to ensure that the models reflect the current state of knowledge. Comparisons between older and newer models should also be attempted a regular basis to evaluate progress in reducing uncertainty. These comparisons should also be incorporated into a systematic review prccess to update the STF models recommended for regulatory applications.

4.2 Recommendation II : Leadership by Risk Assessment Council

EPA's Risk Assessment Council (Council) should ensure that STF research is integrated into EPA's approach to exposure assessment. Specifically, the Council should:

a. Initiate the development of Agencywide guidelines for STF model performance criteria and their acceptability, following methods adopted by OAQPS.

b. Endorse and promote the coordination and use of interagency STF research as part of an effective research strategy for EPA.

4.3 Recommendation III: Establishment of an Early Warning Group

EPA should establish a formal and continuing group of senior scientists and engineers who would be drawn from the Office of Research and Development, the Office of Policy, Planning and Evaluation, and extra-Agency groups. These individuals, representing a number of disciplines, would be charged with identifying potential, emerging, and/or escalating public health and environmental problems. Such a group would, at a minimum, perform the following functions:

a. Survey early warning data sources which can be found from modest refinements to existing chemical, biological and physical data monitoring systems. Such refinements lead to feed forward monitoring, which can determine when new, unregulated or unselected compounds enter a system or when shifts in the distribution of chemicals in the environment occur. Methods for for analyzing such data should be developed.

b. Identify potential human health and environmental risks that are currently not classified as major EPA priorities. The process for identifying such risks should include an examination of social, economic and technological changes that can create new risks, use of existing models and measurement data, and sponsorship of periodic expert workshops to survey expert judgment on trends and risks.

c. Prepare an annual report of potential new problems to be submitted to the Administrator, Deputy Administrator, and the Assistant Administrators. The Assistant Assistant for ORD should ensure that this report is formally considered in each year's research planning process.