An Introductory User's Guide to Risk Assessment Information Sources

EPA

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I. INTRODUCTION

This directory is intended as a sampler of the numerous information sources available for conducting risk assessment. It contains references to EPA databases, models, and staff resources. Key information sources are grouped under each major phase of risk assessment.

Several types of information sources are available for risk assessment. These include databases, data files, tapes, models, manuals, directories, publications, periodicals, and human resources. Databases are the most direct means for accessing large amounts of both quantitative and qualitative data quickly. Models often provide the only means for site-specific analyses. Human resources are invaluable for guidance through the sea of information. In order to simplify this guide, only databases, models, and human resources are included. For listings of other types of information, the Superfund Risk Assessment Information Directory, available through the EPA document retrieval service, is an excellent source.

In selecting the databases and models included here, we have attempted to create a list that represents a good base of information covering several facets of risk assessment. The universe of information sources is overwhelming. This list of databases is a subset of those included in the Superfund Directory cited above. That list was narrowed according to several criteria. Only EPA resources are included. These sources are readily available to EPA staff through the appropriate office. All databases selected are available at this time or will be available soon. Bibliographic databases, which contain only references to other publications, have been excluded from this guide. When several databases contained very similar information, the one with the broadest coverage was selected. Databases with very specialized information were not included.

Chapter II of this guide is organized into four sections corresponding to each step in the risk assessment process: hazard identification, dose-response assessment, exposure assessment, and risk characterization. A listing of databases and/or models, including the name of each information source and a short description, is provided in each section. Additional information on each source is contained in Chapter IV. This information includes a longer description and the EPA office and/or person responsible who can be contacted for additional information.

Throughout the Agency, staff with specialized knowledge are available for consultation on risk assessment problems. Chapter III identifies the key people in both the regional offices and headquarters who can be contacted for guidance on a specific problem and to identify additional information sources.

II. INFORMATION RESOURCES

This chapter summarizes available information resources that might be of use in risk assessment. It is organized into four sections, which follow the major steps in the risk assessment process:

- Hazard identification
- Dose-response assessment
- Exposure assessment
- Risk characterization

Many databases can be used for more than one purpose; therefore, several databases are listed under more than one heading. To keep the lists manageable, the databases are listed only under those headings that they directly address, although the information they contain could also be used for different steps.

HAZARD IDENTIFICATION

Hazard identification addresses the need of establishing what health hazards are present from a specific chemical. The information needed to identify a hazard can be broken down into two categories: physical and chemical properties, and hazard characterization.

Physical and Chemical Properties

The databases listed here contain information on the physical and chemical properties of environmental contaminants.

- OTS Chemical Directory (CHEMD): Provides chemical structures for chemicals in all OTS automated systems.
- Graphical Exposure Modeling System (GEMS): The CHEMEST database contains information on solubility, log P, boiling point, and vapor pressure of various substances.

- Oil and Hazardous Materials--Technical Assistance Data System (OHM-TADS): Contains data gathered on 1,334 materials that have been designated oil or hazardous materials.

- Public Health Risk Evaluation Database (PHRED): Provides chemical, physical, and toxicological data and health-based standards for over 400 chemicals.

- Scientific Parameters for Health and the Environment, Retrieval and Estimation (SPHERE): The ISHOW database contains melting point, boiling point partition coefficient, acid dissociation constant, water solubility, and vapor pressure data for 5,400 chemicals.

- Air Emissions for Treatment, Storage, and Disposal Facilities for Hazardous Waste (TSDF): Will contain the waste stream compositions and physical-chemical properties for TSDFs.

Hazard Characterization

Health hazards from exposure to a contaminant can be characterized based on several different types of data. These databases contain epidemiological and toxicity data.

- Acute Hazards Data: Contains data on the acute toxicity of various chemical substances.

- Air Toxics Clearinghouse: Includes pollutant-specific and source-specific information on toxic air pollutants.

- CSB Existing Chemical Assessment Tracking System (CECATS): Includes information from several sources on chemical identities, health and environmental effects, chemical uses, and market information.

- Environmental Effects/Fate Information System (EEFIS): Contains chemical fate and environmental effects data on chemicals identified for priority testing consideration, chemicals for which test rules have been generated, and chemicals requiring testing under Section 4 of TSCA.

- Integrated Risk Information System (IRIS): Contains results of carcinogenicity bioassays, dose-related responses, toxicity levels, reference doses, and other parameters on about 200 compounds.

- Oil and Hazardous Materials--Technical Assistance Data System (OHM-TADS): Contains information on 1,334 materials designated oil or hazardous material.

- Pesticide Document Management System (PDMS): An index to studies on the properties and effects of pesticides.

- Public Health Risk Evaluation Database (PHRED): Provides chemical, physical, and toxicological data and health-based standards and criteria for over 400 chemicals.

- Studies on Toxicity Applicable to Risk Assessment (STARA): Contains available quantitative toxicological data on all EPA priority pollutants.

DOSE-RESPONSE ASSESSMENT

Dose-response assessment generally involves extrapolation from epidemiological data. This extrapolation may involve factors such as dose duration, dose level, animal versus human studies, or exposure route. The following databases contain dose-response information.

- Genetic Toxicology Division Bioassay System (GTDMIS): Contains the results of numerous biological test systems for detecting carcinogenicity or mutagenicity.

- ORALTOX: Contains acute oral toxicity data for rats, wild birds, and wild mice for about 20,000 chemicals.

- Scientific Parameters for Health and the Environment, Retrieval and Estimation (SPHERE): The Dermal Absorption database contains health effects data for approximately 650 chemical substances. The Genetox database contains mutagenicity data on 3,170 chemicals.

- Studies on Toxicity Applicable to Risk Assessment (STARA): Contains toxicological data on all EPA priority pollutants.

- Integrated Risk Information System (IRIS): Contains results of carcinogenic bioassays, dose-related responses, toxicity levels, reference doses, and other parameters used to control exposure for 200 compounds.

- Dyer EEG Evoked Potential (DEEP): Contains data on the physiological consequences of acute and/or chronic toxicant exposure on nervous system functions.

- Neurotoxicity Data: Contains evaluated neurotoxicity data on many chemicals reviewed by OTS.

- Inhalation Literature: Contains information on inhalation toxicity on 100 chemicals.

EXPOSURE ASSESSMENT

Exposure assessment involves estimating the actual concentration of a chemical to which humans may be exposed. Exposure assessment involves three separate steps: determining the chemical concentration in the environment, determining the population at risk from the contaminant, and determining the exposure route, magnitude, and duration.

Chemical Concentration in Environmental Media

The first step in exposure assessment is to estimate the concentration of the chemical in the environment. Models are often used for this step, but databases can also provide useful information on such factors as chemical concentrations in the ambient environment, quality data for waste streams, or environmental characteristics that may impact a chemical's concentration. For the sake of brevity, only the model names are included in this section. A complete description of the models can be found in Chapter IV.

Databases

- Air Toxics Clearinghouse: Contains pollutant-specific and source-specific information on toxic air pollutants.

- Graphical Exposure Modeling System (GEMS): Contains meteorologic data, geoecology data, stream flow rates, POTW data, and water supply data.

- Pesticide Document Management System (PDMS): An index to studies on the properties and effects of pesticides.

- Storage and Retrieval of Water Quality Information (STORET): Contains water quality data, including aquatic biological data, hydrologic data, and stream reach data.

- Air Emissions from Treatment, Storage, and Disposal Facilities for Hazardous Waste (TSDF): Contains data on TSDFs, including air emission models and dispersion models.

Atmospheric Fate Models

- BOXMDD80
- Climatological Dispersion Model (CDM)
- CRSTER
- Industrial Source Complex (ISC)
- Point Source Discharge--Concentration at a Distance (PTDIS)
- PTMTP
- Point, Area, Line Source Algorithm (PAL)
- RAM
- Texas Episodic Model (TEM)
- Valley

Surface Water Fate Models

- Channel Transport Model (CHNTRN)
- Chemical and Stream Quality Model (TOXIWASP)
- Chemical Transport and Analysis Program (CTAP)
- DYNHYD3
- Enhanced Stream Water Quality Model (QUAL2E)
- Exposure Analysis Modeling System (EXAMS)

- Hydrological Simulation Program--Fortran (HSPF)
- Probabilistic Dilution Model (PDM)
- Metals Exposure Analysis Modeling System (MEXAMS)
- Michigan River Model (MICHRIV)
- Sediment-Contaminant Transport (SERATRA)
- Time-Dependent, Three-Dimensional Transport Model
- Time-Dependent, Three-Dimensional, Variable-Density Hyrodynamic Model
- Toxic Organic Substance Transport and Bioaccumulation Model (TOXIC)
- Transient One-Dimensional Degradation and Migration Model (TODAM)
- Water Quality Analysis Simulation Program (WASP3)
- Water Quality Assessment Methodology (WQAM)
- Water Quality Modeling System for the Great Lakes (WQMSGL)

<u>Unsaturated Zone and Ground Water Fate Models</u>

- MINTEQ
- Pesticide Root Zone Model (PRZM)
- Pesticides Analytical Transport Solution (PESTAN) or Analytical Transient 1, 2, 3--Dimensional Model (AT123D)
- Regulator and Treatment Zone Model (RITZ)
- Seasonal Soil Compartment Model (SESOIL)
- Simulated Waste Access to Ground Water (SWAG)
- Three-Dimensional Plumes in Uniform Ground-Water Flow (PLUMEZD)

Population at Risk

The second step in exposure assessment is estimating the population at risk from the contaminant.

- Graphical Exposure Modeling System (GEMS): Contains 1980 census data for a variety of population statistics.

Exposure Route, Magnitude, and Duration

Parameters useful in assessing exposure routes, magnitudes, and durations include dermal absorption data, oral intake data, toxicological data in dose-duration terms, and bioassay data involving known exposure routes and durations.

- Genetic Toxicology Division Bioassay System (GTDMIS): Contains the testing results of biological tests for detecting carcinogenicity, or mutagenicity.

- Inhalation Literature: Contains information on inhalation toxicity on 100 chemicals.

- Oil and Hazardous Materials--Technical Assistance Data System (OHM-TADS): Contains data on 1,334 materials designated oil or hazardous material.

- Pesticide Document Management System (PDMS): An index on the properties and effects of pesticides.

- Scientific Parameters for Health and the Environment, Retrieval and Estimation (SPHERE): Contains five files on the health and environmental effects of chemical substances.

- Studies on Toxicity Applicable to Risk Assessment (STARA): Contains quantitative toxicological data on all EPA priority pollutants.

RISK CHARACTERIZATION

Risk characterization is the estimation of human health risks or environmental risks from the chemical concentration levels determined in the exposure assessment. Risk characterization is largely the synthesis of information gathered in the first three steps of the risk assessment process.

Human Health Risk

The databases listed here include data on research results on health effects, and testing and regulatory activities. Two models are also listed which provide health risk estimates.

- CSB Existing Chemical Assessment Tracking System (CECATS): Includes information from several sources on health and environmental effects.

- EPA Chemical Activities Status Report (EPACASR): Contains references to chemical substances under review by the EPA.

- General Radiation Health Impact Evaluation: Contains information for assessing health impacts resulting from environmental radiation.

- Integrated Risk Information System (IRIS): Contains results of carcinogenic bioassays, dose-related responses, toxicity levels, reference doses, and other parameters for 200 compounds.

- Oil and Hazardous Materials--Technical Assistance Data System (OHM-TADS): Contains information on 1,334 materials designated oil or hazardous material.

- Physiological Data Acquisition System (PDAS): Contains physiological data from subjects who perform tests while exposed to various pollutants.

- Public Health Risk Evaluation Data Base (PHRED): Contains toxicological data and health-based standards and criteria for over 400 chemicals.

- Studies on Toxicity Applicable to Risk Assessment (STARA): Contains quantitative toxicological data on all EPA priority pollutants.

- Mixture and Systemic Toxicant Risk Model (MSRM): Estimates human health risk from exposure by any route.

- Radionuclide Dose Rate/Risk (RADRISK): Estimates health risk due to inhalation or ingestion of radionuclides.

Environmental Effects:

Environmental effects include changes in aquatic and terrestrial natural resources brought about by exposure to chemical substances. Knowledge of such effects may be important in analyzing chemical migration pathways and potential human exposures; however, knowledge of environmental effects is also important in analyzing the non-human risks of a chemical release. Information that can be found in the following databases includes data on natural resource injuries caused by exposure to chemicals.

- Environmental Effects/Fate Information System (EEFIS): Includes data on chemical fate and environmental effects information.

- Oil and Hazardous Materials--Technical Assistance Data System: Contains data on 1,334 materials designated oil or hazardous material.

- ORALTOX: Contains oral toxicity data for rats, wild birds, and wild mice.

- Scientific Parameters for Health and the Environment, Retrieval and Estimation (SPHERE): Contains data on acute, chronic, bioaccumulative, and sublethal effects of over 2,500 chemical substances on freshwater and marine organisms.

- Studies on Toxicity Applicable to Risk Assessment (STORET): Contains quantitative toxicological data on all EPA priority pollutants.

III. HUMAN RESOURCES

This chapter lists EPA individuals who have been identified as being sources of unique information or advice concerning risk characterizations. These individuals should be contacted only when the data required to characterize risks cannot be found through the traditional information resources.

Several agencies other than EPA may also be useful sources of information on risk assessment. An extensive directory of such agencies is contained in a Public Health Foundation publication entitled Resource Guide for Environmental Health Risk Assessment.

REGIONAL STAFF

Regional Network for Risk Assessment Issues

EPA's Regional Network for Risk Assessment Issues was developed two years ago. The following people are designated by Regional Administrators to serve as primary contacts for participating in agencywide risk assessment initiatives. Many of them also chair their Region's cross-media committee for addressing toxic chemical exposure issues, so they have an overall perspective on risk assessment activities in their Region. Susan Deihl or Earl Bozeman should be contacted for further information, Region IV, FTS 257-3776.

Region I	Tom D'Avanzo Chairman, Toxics Coordinating Committee Air Management Division John F. Kennedy Federal Building Room 2203 Boston, Massachusetts 02203	FTS 223-4864
Region II	Kevin Bricke, Chief Policy and Program Integration Branch 26 Federal Plaza Room 900 New York, New York 10278	FTS 264-4296

	Maria Pavlova, M.D., Ph.D. Office of Emergency and Remedial Response 26 Federal Plaza New York, New York 10278	FTS 264-1918
Region III	Greene A. Jones, Director Environmental Services Division 841 Chestnut Street Philadelphia, Pennsylvania 19106	FTS 597-9378
Region IV	Susan Deihl Risk Assessment Coordinator Office of Policy and Management 345 Courtland Street, N.E. Atlanta, Georgia 30365	FTS 257-3776
Region V	David Dolan Pesticides and Toxic Substances Branch Environmental Services Division 230 South Dearborn Street Chicago, Illinois 60604	FTS 886-5518
Region VI	Jim Bob Sales Hazardous Materials Branch 1201 Elm Street Dallas, Texas 75270	FTS 729-9722
	Jill Lyons Toxics Coordinator Air Branch 1201 Elm Street Dallas, Texas 75270	FTS 729-9187
Region VII	William W. Rice Deputy Regional Administrator 726 Minnesota Avenue Kansas City, Kansas 66101	FTS 757-2800
	Bob Fenemore Air and Toxics Division 726 Minnesota Avenue Kansas City, Kansas 66101	FTS 757-2835
Region VIII	Jim Baker Air and Waste Management Division One Denver Place Denver, Colorado 80202-2413	FTS 564-1524

	Suzanne Wuerthele, Toxicologist One Denver Place Denver, Colorado 80202-2413	FTS 564-1743
Region IX	Arnold Den Senior Science Advisor Office of Policy and Management 215 Freemont Street San Francisco, California 94105	FTS 454-7487
Region X	Gary O'Neal, Director Air & Toxics Division 1200 Sixth Avenue Seattle, Washington 98101	FTS 399-1152
	Dr. Dana Davoli, Toxicologist 1200 Sixth Avenue Seattle, Washington 98101	FTS 399-1757
Office of Air Quality Planning and Standards, RTP		
	Ila Cote, Toxicologist (Mail Drop 12) Office of Air Quality Planning and Standards Research Triangle Park, N.C. 27711	FTS 629-5645

Health Assessment Network

In addition to the Regional Network for Risk Assessment Issues outlined above, there is also a Health Assessment Network, which is a group of EPA staff involved in various aspects of health/risk assessment and have informally agreed to help each other find answers to specific technical questions related to risk assessment. The range of specialties represented in the network is quite broad--e.g., exposure assessment, PCBs, ground-water contamination, general toxicology, and statistics. As of early 1986, there were about 50 EPA staff members in the Health Assessment Network, with representatives from all the regional offices, headquarters, and several field components. There were also about 20 people in the network who represent external organizations such as state health departments, state environmental protection organizations, and private contractors. For more information about the Health Assessment Network, contact Suzanne Wuerthele, Region VIII, FTS 564-1743.

Air Toxics

The following EPA Regional personnel are designated contacts for air toxics questions (only names and telephone numbers are given below; the addresses for regional offices are given above for the risk assessment contacts).

Region I	Margaret McDonough (617) 223-4870; FTS 223-4870
	Beth Hasset (617) 223-4880; FTS 223-4880
Region II	Bob Kelly (212) 264-2517; FTS 264-2517
Region III	Iz Milner (215) 597-9090; FTS 597-9090
	Paul Racette (215) 597-9009; FTS 597-9009
Region IV	Doug Cook (404) 347-2864; FTS 257-2864
Region V	Harriet Croke (312) 353-6009; FTS 353-6009
Region VI	Jill Lyons (214) 767-9187; FTS 729-9187
Region VII	Bob Chanslor (913) 236-2893; FTS 757-2893
Region VIII	Dewitt Baulch (303) 293-1761; FTS 564-1761
Region IX	Tim Smith (415) 974-8219; FTS 454-8219
Region X	Dana Davoli (206) 442-1757; FTS 399-1757

HEADQUARTERS STAFF

Risk Assessment Council

The Risk Assessment Council was organized to provide executive oversight of the development, review, and implementation of risk assessment policy.

Chairman:	John A. Moore Office of Pesticides and Toxic Substances
Coordinator:	Donald Barnes Office of Research and Development (202) 382-2897

Risk Assessment Forum

The Risk Assessment Forum is made up of 10 senior agency scientists. Its objective is to promote consensus on risk assessment issues and ensure incorporation into risk assessment guidance.

Chairman:	Peter W. Preuss Director, Office of Health and Environmental Assessment
Executive Secretary:	Dorothy Patton Office of Research and Development (202) 475-6743

Risk Management Council

The Risk Management Council was organized to provide executive oversight of the development, review, and implementation of risk management policy.

Chairman:	Lee Thomas Administrator
Coordinator:	Deborah Taylor Office of the Administrator (202) 382-7960

OTS Chemical Assessment Desk

The OTS Chemical Assessment Desk is an outreach service to other EPA offices and regions. It provides information on risk assessment activities for chemicals evaluated in the OTS Existing Chemicals Program. The Desk also provides estimates of chemical toxicity and environmental fate based on structure-activity relationships in the absence of data, and offers assistance in identifying related risk assessment activities in other EPA program offices. The Chemical Assessment Desk can be reached through Terry O'Bryan, FTS 8-382-3483, (202) 382-3483.

Office of Information Resources Management: Risk Assessment/Risk Management Bulletin Board

The Office of Information Resources Management has established a risk assessment and risk management Bulletin Board on EPA's electronic mail (E-mail) system. Anyone in EPA with access to E-mail can post messages on the Bulletin Board and read messages posted by others. The Bulletin Board can be used to post notices of upcoming conferences, workshops, and other events; request assistance from others on specific risk assessment or risk management problems; inform others of useful information; and, in general, promote further communication regarding risk-related matters. For assistance in posting announcements or reading entries on the Bulletin Board, contact Electronic Mail User's Support at FTS 8-382-5639 ro Earl Bozeman, Region IV, FTS 8-257-3776.

Office of Research and Development

Peter W. Preuss, Ph.D.
Director, Office of Health and Environmental Assessment
FTS 8-382-7315

William Farland, Ph.D.
Office of Health and Environmental Assessment
FTS 8-382-5898
(NOTE: Contact for cancer/mutagenicity/reproductive effects risk assessment questions)

Michael A. Callahan, Ph.D.
Office of Health and Environmental Assessment
FTS 8-475-8909
(NOTE: Contact for exposure assessment questions)

Lester Grant, Ph.D.
Environmental Criteria and Assessment Office
FTS 8-629-4173
(NOTE: Lester Grant is located in Region IV, Hwy 54 and Alex Road, Research Triangle Park, NC, 27711)

Chris DeRosa
Environmental Criteria and Assessment Office
FTS 8-684-7534
Commercial (513) 569-7534
(NOTE: Chris DeRosa is located in Region V, 26 West St. Clair Street, Cincinnati, OH 45268)

Office of Emergency and Remedial Response

Craig D. Zamuda, Ph.D.
Policy Analysis Staff
FTS 8-382-2201

Office of Waste Programs Enforcement

Sheryl Sterling
Chief, Health Sciences Section
FTS 8-382-5646

Office of Pesticide and Toxic Substances

Arnold Edelman
Chemical Activity Coordination Group
FTS 8-382-2249

Ted Farber
Liaison with FDA on Fish Contamination Issues
(202) 557-7351

Office of Solid Waste

Reva Rubenstein
Chief, Health Assessment Section
(202) 382-5219

Art Glazer
Chief, Storage/Incineration Permit Assistance Section
(202) 382-4652

Terry Grogan
Chief, Land Disposal Permit Assistance Section
(202) 382-4740

Office of Air and Radiation

Robert Kellam
Section Chief, Pollutant Assessment Branch
Research Triangle Park, NC
(919) 541-5646; FTS 8-629-5646

IV. REFERENCES FOR DATABASES AND MODELS

This chapter contains more complete descriptions of the databases and models cited in Chapter II. It is divided into two main sections: databases and models. Some of the items included in this chapter as databases (e.g., IRIS) are actually ancillary automated systems which facilitate the research and manipulation of data; these systems can be distinguished from sources of data by their description as "indexing," "tracking," or "search system" under "Type." After the description of each database, references for additional information are given. For most of the databases, the EPA office where the database resides and a responsible person are provided. These descriptions are reproduced from the Superfund Risk Assessment Information Directory.

The list of databases and models is far from exhaustive. The databases were identified through EPA's "Information Systems Inventory," an agencywide compilation of databases. These databases have been selected because they have been identified as having the primary purpose of risk assessment, and because together they cover a wide range of topics. There are several additional databases, some of which are very narrow in scope, which may be more applicable or useful for a given situation. The models chosen here are accepted, commonly used environmental fate and transport and exposure assessment models. As with the databases, numerous additional models exist that may be better suited to a particular problem.

DATABASES

Acute Hazards Data

Subject: Acute Toxicity of Substances

Content: This microcomputer-based database on the acute toxicity of various chemical substances has been developed by OTS in support of an agencywide activity following the Bhopal, India tragedy. This database will be used to develop materials to circulate to states and localities concerning a list of 400 chemicals identified by EPA as being potentially of concern if released to the environment.

Holder: Economics and Technology Division, U.S. EPA

Responsible Person: Nilesh Patel

FTS Phone: 8-382-3718

Air Emissions from Treatment Storage and Disposal Facilities for Hazardous Waste (TSDF)

Subject: Air Emissions

Type: Non-bibliographic

Content: The TSDF, which is currently under development, will contain information about industrial facilities which treat, store, or dispose of hazardous waste. Data to be compiled in TSDF include company names, locations, and descriptions, the size of each site, waste stream compositions, and physical-chemical properties. In addition, air emission models and dispersion models will be included. The TSDF will be used to generate air emission inventories to support future air pollution regulation.

Holder: Office of Air and Radiation

Responsible Person: Gene Smith

FTS Phone: 8-629-5571

Air Toxics Clearinghouse

Subject: Toxic Air Pollutants

Type: Bibliographic and information search

Content: This database was developed to help exchange information among state and local environmental agencies and the EPA. The contents include over 60,000 records on subjects like: control programs, correspondence, publications, reports, and data of states' developed and developing programs.

Time Span: Varies with file

Updating: Varies with file

Holder: Office of Air Programs, U.S. EPA

Online Service: Government access through Account with EPA. On EPA IBM Mainframe. Private access through NTIS.

Contact: Dave Patrick or Karen L. Blanchard
(919) 541-5519

CSB Existing Chemical Assessment Tracking System (CECATS)

Subject: Chemical-Specific Hazard Information

Type: Document Tracking

Content: CECATS is an automated document tracking system designed to aid the Chemical Screening Branch (CSB) in reviewing data on existing chemicals and selecting those substances that require additional attention by the Office of Toxic Substances (OTS). The system provides storage, retrieval, verification trails, data manipulation, and report generation for information on existing chemicals associated with: TSCA Section 8(e) submissions, For Your Information (FYI) submissions, Chemical Hazard Information Profiles (CHIP), Pre-Chip screenings, and Substitute Hazard Profiles. These sources provide information on chemical identities, health and environmental effects, chemical uses, and market information. Information on the status of a chemical within OTS is also provided.

Holder: Office of Toxic Substances

Responsible Person: James Darr

FTS Phone: 8-382-3470

Dyer EEG Evoked Potential (DEEP)

Subject: Nervous System Health Effects

Type: Non-bibliographic

Content: Data are maintained on the physiological consequences of acute and/or chronic toxicant exposure on nervous system functions

Holder: Office of Health Research

Responsible Person: Robert Dwyer

FTS Phone: 8-629-2760

EPA Chemical Activities Status Report (EPACASR or CASR)

Subject: Chemistry

Type: Reference (Bibliographic)

Content: This database contains more than 19,000 references to over 8,000 chemical substances review or under review by the U.S. EPA in the course of its regulatory activities and scientific research. A summary of EPA activities is provided with each named substance.

Time Span: Up to February 1984

Updating: It is not updated

Responsible Person: Doug Sellers

Telephone: (202) 382-2320

Environmental Effects/Fate Information System (EEFIS)

Subject: Chemical Fate; Environmental Effects

Type: Non-bibliographic (Textual-Numeric)

Content: EEFIS provides user-friendly, menu-driven access through any IBM-compatible personal computer to chemical fate and environmental effects information on selected chemicals. The database contains a variety of information resources, published and unpublished, such as journal articles, correspondence, tables, FYI studies submitted to EPA by industry, non-CBI Section 8(d) studies, and Section 4 information. EEFIS contains chemical fate and environmental effects data (1) on chemicals identified for priority testing consideration by the interagency testing committee; (2) on chemicals for which EPA's Test Rules Development Branch has internally generated tests rules or has received requests from other program offices to promulgate test rules; and (3) generated as a result of EPA's required testing under Section 4 of TSCA.

Holder: Office of Toxic Substances, Existing Chemical Assessment Division

Responsible Person: John D. Walker

Telephone: (202) 475-8160

General Radiation Health Impact Evaluation

Subject: Radiation Exposure Assessment

Type: Non-bibliographic

Content: This system is used to assess health impacts resulting from environmental radiation from sources such as radon in surface water, drinking water, and air. Information in the system is also used to assess health effects of gamma radiation levels measured by TLD dosimeters.

Holder: Office of Radiation Programs

Responsible Person: D. Norwood

FTS Phone: 8-534-7615

Genetic Toxicology Division Bioassay System (GTDMIS)

Subject: Health Effects

Type: Non-bibliographic

Content: This system contains the results of testing various chemical compounds in numerous biological test systems for detecting carcinogenicity or mutagenicity. The results are entered from in-house research (HERL-Genetic Toxicology Division), National Cancer Institute reports, and other published genetic toxicology literature.

Holder: Office of Health Research

Responsible Person: Mike Waters

FTS Phone: 8-629-2537

Graphical Exposure Modeling System (GEMS)

Subject: Environmental Fate and Transport; Populations at Risk

Type: Non-bibliographic

Content: This database contains 12 datasets and fosters rapid access to 11 environmental fate and transport models designed to assess risks from waste sites which are migrating through various environmental media. The GEMS fate and transport models are discussed in the next section of this chapter. The data sets include:

CHEMSET Validation. Includes information on solubility, log P, boiling point, and vapor pressure of various substances.

ECONOMIC CENSUS 1977. Contains information on manufacturers, industry, and transportation from 1977.

GEOCOLOGY DATABASE. Contains county level data from selected areas on agriculture, climate, vegetation, soils, population, water quality, and wildlife.

GAGE. Contains stream flow rates from approximately 99,500 stations throughout the United States.

IFDPIR. Contains facility data for approximately 28,000 dischargers, excluding POTWS.

IFDIND. Contains facility data for approximately 12,000 discharges who discharge through other facilities, usually POTWS.

MARF 1980 Census. Contains a variety of location identification information, population counts by race, the numbers of families for all 50 states.

METEOROLOGICAL DATA. Contains data for 394 weather stations in the continental United States.

POTWS. Contains 1982 survey data from 33,000 publicly owned treatment works in the United States.

REACH. Contains stream reach information, including cataloging unit, segment number, and location for approximately 68,000 reaches throughout the country.

WATER SUPPLY. Contains the number of surface water utilities, the total population served, the number of intake points, and the number of STORET water quality stations associated with surface water utilities.

Holder: Office of Toxic Substances
Exposure Evaluation Division

Telephone: (202) 382-3928

Inhalation Literature

Subject: Inhalation toxicity

Type: Non-bibliographic

Content: This microcomputer-based compilation contains information from the open literature on inhalation toxicity. It includes approximately 500 records on 100 chemicals.

Holder: Health and Environmental Review Division

Responsible Person: Ernest Falke

FTS Phone: 8-382-3430

The Integrated Risk Information System (IRIS)

Subject: Risk characteristics of chemicals

Type: Search system

Content: IRIS contains results of carcinogenic bioassays, dose-related responses, toxicity levels, reference doses, and other parameters used to control exposure. The system is organized on a chemical basis and the user can call up a chemical by name and review all material pertinent to it. IRIS should be on-line in October or November of 1986, and will contain authoritative information on about 200 compounds. Designed as an electronic loose-leaf notebook, IRIS can be accessed through commercial E-mail lines, and provides users with the ability to access, copy, and print information from the database, while data entry access is limited to maintain the integrity of the file.

Holding Office: Office of Health and Environmental Assessment

Responsible People: Mary Wigginton (FTS 8-382-7315) for status and access information; Jeffrey Swartout (FTS 8-684-7811) for scientific issues and accuracy of reference doses

Neurotoxicity Data

Subject: Neurotoxicity evaluations

Type: Bibliographic and Non-bibliographic

Content: The Toxic Effects Branch of OTS is developing this microcomputer-based database of evaluated neurotoxicity data. This database will cover the many chemicals reviewed by OTS for neurotoxicity under the Toxic Substances Control Act (TSCA). The database consists of records at the chemical level, individual article level, and at the experimental observational level. The database should be implemented by summer 1986.

Holder: Health and Environmental Review Division

Responsible Person: Michael Cimino

FTS Phone: 8-382-3451

Oil and Hazardous Materials--Technical Assistance Data System (OHM-TADS)

Subject: Environment; Toxicology

Type: Non-bibliographic (Textual-Numeric)

Content: A database containing data gathered from published literature on 1,334 materials that have been designated oil or hazardous materials. Provides technical support for dealing with potential or actual dangers resulting from the discharge of oil or hazardous substances. Up to 126 data fields, some textual and some numeric, may be present for each record (i.e, one material). A record includes identification of the substance (Chemical Abstracts Service registry number, common and trade names, and chemical formula), physical properties, uses, toxicity, handling procedures, and suggested methods for disposing of spilled materials. Emphasis is placed on the effects of these substances on water quality.

Updating: About 50 new entries each year.

Producer: U.S. EPA

On-line Service: Chemical Information System, Inc. (CIS); Information Consultants, Inc. (ICI)

Oraltox

Subject: Acute Oral Toxicity

Type: Non-bibliographic

Content: Oraltox contains acute oral toxicity data for rats, wild birds, and wild mice. The data are sorted according to CAS number, chemical name, and the number of carbons in the chemical formula. All of the data are from literature, with rat toxicity data taken from the Registry of Toxic Effects of Chemical Substances and bird and mice data taken from literature by the U.S. Fish and Wildlife Service. Data for about 20,000 chemicals are listed in Oraltox.

Holder: Office of Toxic Substances

Responsible Person: Richard Clements

FTS Phone: 8-382-4270

OTS Chemical Directory (CHEMD)

Subject: Physical-Chemical Properties

Type: Non-bibliographic

Content: CHEMD will provide a common storage and retrieval capability for chemical structures for chemicals in all OTS automated systems. It will provide chemical structure and substructure search features with sophisticated graphics capabilities.

Holder: Office of Toxic Substances

Pesticide Document Management System (PDMS)

Subject: Pesticides

Type: Bibliographic

Content: The PDMS database is an on-line index to some 200,000 studies of the properties and effects of

pesticides. These are mostly unpublished documents, submitted by the pesticide industry to support regulatory decisions by the Office of Pesticide Programs. Microform copies of all indexed documents are maintained in OPP offices. The index supports searching by chemical, subject, and a wide range of other bibliographic and non-bibliographic attributes of each document. Due to widespread claims of data confidentiality by their submitters, ready access to PDMS documents is restricted to EPA staff cleared for access to FIFRA confidential business information.

Holder: Office of Pesticide Programs

Responsible Person: John Carley

FTS Phone: 8-557-3240

Physiological Data Acquisition System (PDAS)

Subject: Health Effects

Type: Non-bibliographic

Content: The PDAS contains real-time physiological data (e.g., pulmonary function, heart, and stress measurements) from subjects who perform various tests while enclosed in chambers exposing them to various levels of pollutants. One of the pollutants studied is ozone.

Holder: Office of Health Research

Responsible Person: John O'Neil

FTS Phone: 8-629-2602

Public Health Risk Evaluation Database (PHRED)

Subject: Chemical, physical, and toxicological data and health-based standards

Type: Non-bibliographic with source citations

Content: This personal computer software package is designed to provide chemical, physical, and toxicological data and health-based standards and criteria for over 400 chemicals that may be found at Superfund sites. The package is intended to accompany the Superfund Public Health Evaluation Manual (Office of Solid Waste and Emergency Response Directive 9285.4-1) which is also the source of most of the data. More detailed information about specific types of data in the database can be found in the manual, and footnotes and data sources are included throughout the data.

Holder: Office of Emergency and Remedial Response, Policy Analysis Staff

Responsible Person: Craig Zamuda

FTS Phone: 8-382-2201

Scientific Parameters for Health and the Environment, Retrieval, and Estimation (SPHERE)

Subject: Biomedicine; Chemistry-Properties; Environment; Toxicology

Type: Reference (Bibliographic); Non-bibliographic (Textual-Numeric)

Content: Contains five files of information on health and environmental effects of chemical substances. Data are extracted from the published literature.

AQUATIC INFORMATION RETRIEVAL DATABASE (AQUIRE). Contains data on acute, chronic, bioaccumulative, and sublethal effects of over 2,500 chemical substances on freshwater and marine organisms (excluding bacteria, birds, and aquatic mammals).

DERMAL ABSORPTION DATABASE. Contains information on the qualitative and quantitative health effects of approximately 650 chemical substances administered to humans and test animals via the dermal route.

ENVIROFATE. Contains information on the environmental fate or behavior (i.e., transport and degradation) of chemicals released into the environment. Chemicals selected for inclusion are produced in quantities exceeding 1 million pounds per year. Data, extracted from published literature, include environmental transformation rates (e.g., biodegredation, oxidation, hydrolysis) and physical and chemical properties (e.g., water solubility, vapor pressure).

GENETOX. Contains mutagenicity information on 3,170 chemicals that were tested against 38 biological systems. Data are extracted from published literature.

INFORMATION SYSTEM FOR HAZARDOUS ORGANICS IN WATER (ISHOW). Contains melting point, boiling point, partition coefficient, acid dissociation constant, water solubility, and vapor pressure data for more than 5,400 chemicals.

Time Span: 1970-present

Updating: Periodically, as new data become available

Producer: U.S. EPA

On-line Service: Chemical Information System, Inc. (CIS; Information Consultants, Inc. (ICI)

Storage and Retrieval of Water Quality Information (STORET)

Subject: Water Quality Data

Type: Non-bibliographic

Content: STORET contains water quality data used by state and EPA analysts in making water pollution control decisions (e.g., issuing NPDES permits, establishing water quality standards for toxic pollutants, evaluating the effectiveness of regulatory programs, and assessing concentrations of toxic pollutants). Data contained in STORET include aquatic biological data, hydrologic data, stream reach data, and other related information.

Approximately 60 million observations of water quality parameters measured at about 200,000 monitoring sites in the United States are included in the database, along with information on how and where the data were obtained.

Holder: Office of Water

Responsible Person: Phillip Lindestruth

FTS Phone: 8-382-7220

Studies on Toxicity Applicable to Risk Assessment (STARA)

Subject: Toxicological Data

Type: Non-bibliographic

Content: This system contains available quantitative toxicological data on all EPA priority pollutants (water quality and air lists). Data are extracted from peer-reviewed studies which are screened for appropriateness for human health risk estimation. Related software procedures (WYLBUR EXEC) allow generation of formatted tables of the original data, tables of data in human equivalent (dose-duration) terms, and graphs of severity versus dose and duration.

Holder: Office of Health and Environmental Assessment

Responsible Person: Richard Hertzberg

FTS Phone: 8-684-7582

MODELS

Atmospheric Fate Models

BOXMDD80

- Contains population retrieval program
- Applicable primarily to regions containing many diffuse emission sources
- Steady-state, Gaussian distribution
- Exposure routine is included
- Available on GEMS

Reference: Hanna, 1972
Contact for access to GEMS: Loren Hall, EPA
(202) 382-3931

Climatological Dispersion Model (CDM)

- Long-term seasonal or annual
- Point or area sources
- Gaussian plume model
- Simulates non-conservative pollutants
- Can simulate turbulence over urban areas
- Outputs long-term average concentrations at user-specified receptors
- Requires stability array data
- FORTRAN V program language; has been implemented on the UNIVAC 1110
- 22K bytes storage required

- Software available as part of UNAMAP package for $420
- A modified version (CDMQC) includes calibration of individual point and area source contribution lists and of averaging time transformations.

Documentation: Busse and Zimmerman, 1976
Software: Computer Products, NTIS, Springfield, Virginia 22161

CRSTER

- Modified steady state Gaussian Plume algorithm.
- Estimates ground level concentrations resulting from up to 19 colocated elevated stack emissions.
- Terrain adjustment can be made.
- Prints out the highest and second highest 1-hour, 3-hour, and 24-hour concentrations; also gives annual mean concentration at 180 receptors.

Documentation: U.S. EPA, 1977.

Industrial Source Complex

- Long-term or short-term, point area, or line sources, single or multiple sources.
- Models gravitational settling of particulates, providing deposition.
- Release rates can be varied as a function of time.
- Not applicable to complex terrain.
- May provide overly conservative short-term maximum values for calm wind conditions.
- Requires stability array data.
- Extensive input data required to make use of sophisticated features.
- FORTRAN IV program language, has been implemented on UNIVAC 140.

- Approximately 65 K bytes storage required.
- Available through GEMS.

Documentation: Bowers et al. 1979
Software: Computer Products, NTIS, Springfield, Virginia 22161

Point Source Discharge--Concentration at a Distance (PTDIS)

- Steady-state Gaussian plume model
- Point-source
- Accommodates limit to upward vertical mixing.
- Short-term
- Assumes conservative pollutant
- Produces estimates of hourly concentrations at a user-selected downwind distance.
- Available through GEMS
- FORTRAN IV Program, applicable to wide range of computers; has been implemented on UNIVAC 1110
- Approximately 12 K bytes memory required
- Software available as part of UNIMAP package, for $420

References: Turner and Busse, 1973, General Software Corporation, 1982
Software: Computer Products, NTIS, Springfield, Virginia 22161

Point Source Discharge--Maximum Concentration (PTMAX)

- Steady-state Gaussian plume model
- Point-source
- Short-term

- Assumes conservative pollutant
- Produces maximum hourly concentrations for each stability and wind speed, location of maximum concentration
- Available through GEMS
- FORTRAN IV Program, applicable to wide range of computers; has been implemented on UNIVAC 1110
- Approximately 12 K bytes memory required
- Software available as part of UNIMAP package, for $420

References: Turner and Busse, 1973, General Software Corporation, 1982
Software: Computer Products, NTIS, Springfield, Virginia 22161

PTMTP

- Estimates the concentration from a number of point sources at a number of arbitrarily located receptors at/or above ground level.
- Hourly meteorological data are used.
- Hourly concentrations and averages over any averaging time from 1 to 24 hours can be obtained.
- Downwind and crosswind distances are determined for each source receptor pair.

Documentation: Turner and Busse, 1973

Point, Area, Line Source Algorithm (PAL)

- A short-term Gaussian steady-state algorithm.
- Estimates concentrations of stable pollutants for point, line, and area sources.
- Valuable emission rate along line source can be included.

- Intended for smaller scale analysis such as for shipping centers, airports, and single plants.
- Hourly concentrations are estimated.

Documentation: Peterson, 1978.

RAM

- A Gaussian plume short-term multiple source air quality algorithm.
- Estimate concentrations of stable pollutants form urban point and area sources.
- Hourly meteorological data are used.
- Allows determination of downwind receptor locations to ensure good area coverage with minimum number of receptors.

Documentation: Turner and Novak, 1978.

Texas Episodic Model (TEM)

- Steady state model
- Point or area sources
- Short-term--10 minutes to 24 hours
- Produces maximum and average concentrations over time periods selected by user.
- User can select up to 2,500 downwind receptor points, according to an automatic or specific grid array
- Handles nonconservative pollutants
- Up to 24 meterologic scenarios can be input for a single run.
- FORTRAN program applicable to a wide range of computer types; has been implemented on Burroughs 6810/11

- Requires approximately 26 K bytes memory.
- Engineering, meteorology, atmospheric transport background useful.

Reference: Christiansen, 1976

Valley

- Short- or long-term
- Simulates plume impaction in complex terrain
- Provides screening estimates for worst-case short-term concentrations
- Provides annual average concentrations
- 112-receptor grid
- Accommodates nonconservative pollutants
- Requires stability array data for long-term option
- Requires user-input worst-case meteorological data for short-term screening option
- May require careful analysis of output by experienced air quality modeler
- FORTRAN V program, applicable to wide range of computers
- Approximately 13 K bytes memory required
- Software available as part of UNAMAP series, for $420

Documentation: Burt, 1977
Software: Computer Products, NTIS, Springfield, Virginia 22161

Channel Transport Model (CHNTRN)

- Time-varying, 1-dimensional model
- Models organic pollutants
- Second-order decay mechanisms

- Models rivers, lakes, estuaries, and coastal waters
- Can be coupled with a hydrodynamic model, CHNHYD, for estimation of flow dynamics where such data are not available
- Requires extensive data input, and extensive set-up time
- Has not been field tested and documentation is currently under review
- FORTRAN IV program language
- Applicable to IBM 3933 computer, and others

Reference: Yeh 1982
Documentation: Dr. G.T. Yeh
Environmental Sciences Division
Oak Ridge National Laboratory
P.O. Box X
Oak Ridge, Tennessee 37830
(615) 574-7285

Chemical and Stream Quality Model (TOXIWASP)

- Time-varying, 3-dimensional model
- Comprehensive second-order decay kinetics for organic pollutants
- Models rivers and estuaries and it can be applied to lakes
- Very data-intensive model
- Applicable to IBM 370 or PDP 11/70
- Software in FORTRAN IV; requires 64 K byte memory
- Requires 150-300 man-hours for set-up

Documentation and Software: Robert Ambrose
Center for Water Quality Modeling
U.S. EPA
Athens, Georgia 30612
(404) 546-3546

Chemical Transport and
Analysis Program (CTAP)

- Steady state, 3-dimensional compartmental model
- Complex computer program
- Contains comprehensive second-order decay kinetics for organics (most models only have first-order kinetics)
- Models organic chemicals
- Suitable for freshwater, non-tidal aquatic systems
- Requires extensive data input
- Has been incorporated into EPA-OTS GEMS system
- An estimated 350 man-hours required for installation and set-up, assuming all data are readily available
- Well documented and recommended for use over most other models
- Available on magnetic tape for installation on mainframe or small computers (e.g., PDP-11 or HP 3000); batch version requires 64K bytes memory at a minimum, more for complex modeling
- Also available in interactive version, requiring 164 K bytes memory plus 2 K bytes for each chemical and 2.5 K bytes for each environment

Reference: Burns et al. 1982

Documentation: ORD Publications, Center for Environmental Research Information
U.S. EPA
Cincinnati, Ohio 45268
513-684-7562; or
Center for Water Quality Modeling
Environmental Research Laboratory
U.S. EPA
Athens, Georgia 30613
404-546-3585

DYNHYD3

- A simple 2-dimensional hydrodynamic model capable of handling variable tidal cycles, wind, and unsteady inflows
- Updated from the Potomac Dynamic Estuary Model (DEM)
- Has the ability to produce an output file that can be liked with WASP3 (described near the end of this section) to supply the flows and volumes to the water quality model
- Designed for the DOS environment on the IBM PC XT/AT family of microcomputers and compatible systems
- Language: FORTRAN 77
- Approximate run time using sample data sets: 16 minutes

Contact: Center for Water Quality Modeling
Environmental Research Laboratory
U.S. EPA
Athens, Georgia 30513
404-546-3585

Enhanced Stream Water Quality Model (QUAL2E)

- A steady state model for conventional pollutants in branching streams and well mixed lakes
- Includes conservative substances, temperature, coliform bacteria, biochemical oxygen demand, dissolved oxygen, nitrogen, phosphorus, and algae
- Widely used for waste load allocation and permitting in the United States and other countries
- Designed for the DOS environment on the IBM PC XT/AT family of microcomputers and compatible systems
- Approximate run time observed using sample data sets: 1 minute

Contact: Center for Water Quality Modeling
Environmental Research Laboratory
U.S. EPA
Athens, Georgia 30613
404-546-4585

Exposure Analysis Modeling System (EXAMS)

- Subject: Synthetic Organic Chemicals in Aquatic Systems
- Simulation model
- 1-, 2-, or 3-dimensional
- Runs analyses of initial conditions, time variations, steady state analysis
- Uses a set of fundamental process models that accept standard chemical parameters and limnological data as input parameters
- DAC-VAX family of computers and IBM PC compatibles
- FORTRAN 77 standard
- Available through GEMS

Contact: Dr. Lawrence Burns
Office of Environmental Processes and Effects Research
Environmental Research Laboratory
Athens, Georgia (404) 546-3511

Hydrological Simulation Program--Fortran (HSPF)

- Time-varying, 1-dimensional model
- Designed for year-round simulation
- Models organic pollutants
- Second-order decay mechanisms
- Models non-tidal rivers and streams and mixed lakes
- Has been used on IBM 370 series computers
- Requires extensive data input
- Most suitable to minicomputers (e.g., HP 3000, PRIME, Harris) as model utilizes direct access input-output, which can be costly on mainframe computers

- Requires 250 K bytes of overlay-type storage

Reference: Johanson et al. 1980
Software: Center for Water Quality Modeling
Environmental Research Laboratory
U.S. EPA
Athens, Georgia 30613
404-546-3585

Probabilistic Dilution Model (PDM)

- Estimates the percent of time a given concentration level may be exceeded in receiving streams

  Model estimates based on statistical distribution of daily volume flows and on solution of mass balance dilution evaluation

- Contains averages of mean and low flows of streams in major river basins of United States, broken down by direct and indirect dischargers and standard industry classification codes

- Designed for use on personal computers

Holding Office: Office of Toxic Substances
Responsible Person: Karen Hammerstrom
FTS Phone: 8-382-3896

Metals Exposure Analysis
Modeling System (MEXAMS)

- Steady state, 3-dimensional compartmental model

- Complex computer program

- A combination of two models (MINTEQ and EXAMS) designed for modeling of metal loadings

- Suitable for freshwater, nontidal aquatic systems

- Complex metal dynamics requiring extensive data input

- Can be used with mainframe or small (e.g., PCP 11/70 or HP 3000 computers)

- Interactive format
- Contains database with thermodynamic properties of seven metals

Further information: Yasuo Onishi
Battelle, Pacific Northwest Laboratories
Richland, Washington 99352
509-376-8302

Documentation: Center for Water Quality Modeling
Environmental Research Laboratory
U.S. EPA
Athens, Georgia 30613
404-546-3585

Michigan River Model (MICHRIV)

- Steady-state, 1-dimensional model
- Computer program written in FORTRAN
- Similar to SLSA but can model more than one reach
- Intended for metals
- Models rivers and streams
- Easy to set up and use
- Requires minimal computer programming

Reference: Delos et al. 1984
Technical Assistance
Available from: Bill Richardson
U.S. EPA
Environmental Research Laboratory-Duluth
Large Lakes Research Station

Sediment-Contaminant Transport (SERATRA)

- Time-varying, 2-dimensional model (longitudinal and vertical)
- Complex sediment transport mechanisms

- Second-order decay mechanisms for organic pollutants
- Models rivers and lakes
- Requires extensive data input
- Computer program written in FORTRAN preprocessor language FLECS, in batch mode
- Has been field tested and is available for use
- Requires an estimated 750 man-hours for set-up, assuming all required data are readily available

References: Onishi and Wise 1982a
Onishi and Wise 1982b

Documentation: ORD Publications
Center for Environmental Research Information
U.S. EPA
Cincinnati, Ohio 45268
413-684-7562

Technical Assistance: Robert Ambrose
U.S. EPA, Athens Env. Research Lab
Center for Water Quality Modeling
Athens, Georgia 30613
404-546-3546

Time-Dependent, Three-Dimensional Transport Model

- Calculates hydrodynamic transport of conservative and non-conservative substances in surface water bodies
- Estimates time-dependent concentrations
- User-specified options permit application to conservative substances (e.g., chloride) and non-conservative substances (e.g., suspended solids)

Holding Office: Office of Environmental Processes and Effects Research

Responsible Person: J.F. Paul

FTS Phone: 8-838-5087

Time-Dependent, Three-Dimensional, Variable-Density Hydrodynamic Model

- Estimates the movement of pollutants in thermal discharges in harbors, bays, lake basis, entire lakes, estuaries, marine coastal areas, etc.
- Calculates velocities, temperatures, and salinity
- Results of model can be used as input to a separate transport model
- Various user-specified versions to consider the receiving waters in different ways (e.g., water surface treated as a rigid lid or a free-surface, or bottom boundary condition specified as no-slip or slip)

Holding Office:	Office of Environmental Processes and Effects Research
Responsible Person:	J.F. Paul
FTS Phone:	8-838-5087

Toxic Organic Substance Transport and Bioaccumulation Model (TOXIC)

- Quasi-dynamic, 3-dimensional compartment model
- Program language is FORTRAN
- Complex biological uptake mechanisms
- Models pesticides in reservoirs and aquatic impoundments
- Only time-varying functions for loading, not flows
- Good for biological accumulation but lacking in chemical fate mechanisms
- Applicable to IBM 370 and 750 Prime systems
- FORTRAN program in batch mode
- User support is limited; no user manual is available

Reference: Schnoor et al. 1981
Software: Jerry Schnoor
Civil and Environmental Engineering
Energy Engineering Division
University of Iowa
Iowa City, Iowa 52248
319-353-7262

Transient One-Dimensional Degradation and Migration Model (TODAM)

- Time varying, 1-dimensional model
- Second-order decay mechanisms
- Models river and estuarine systems
- Exterior hydrodynamic model (e.g., EXPLORE) is required to provide channel and flow characteristics to TODAM
- Requires extensive data input
- Complex FORTRAN program, written in the preprocessor language FLECS, or in FORTRAN IV
- Applicable to VAC or PDC 11/70 computers (batch mode)
- TODAM has been applied; however documentation is currently under review; release date unknown

Reference: Onishi et al. 1982
Further Information: Yasuo Onishi
Battelle-Pacific Northwest Laboratories and ICF Northwest
Richland, Washington 99352
509-376-8302

Water Quality Analysis Simulation Program (WASP3)

- A generalized modeling framework for contaminant fate and transport in surface waters
- Based on a flexible compartment modeling approach, which allows WASP3 to be applied in one, two, or three dimensions

- Problems that have been studied using WASP3 include biochemical oxygen demand-dissolved oxygen dynamics, nutrients and eutrophication, bacterial contamination, and toxic chemical movement
- Can be used with subroutines selected from a library or written by user (e.g., TOXIWASP described earlier in this section)
- Designed for the DOS environment on the IBM PC XT/AT family of microcomputers and compatible systems
- Language: FORTRAN 77

Contact: Center for Water Quality Modeling
Environmental Research Laboratory
U.S. EPA
Athens, Georgia 30613
404-546-3585

Water Quality Assessment Methodology (WQAM)

- Steady-state, 1-dimensional model
- Requires only desk-top calculations
- Provides canonical information
- Models, lakes, rivers, and estuaries
- Easy to set up and use
- No computer programming needed; requires only hand calculator
- Recommended if time, costs, or information are restrictive

Reference: Mills et al. 1982
Documentation: ORD Publications
U.S. EPA, Cincinnati, Ohio 45268
513-684-7562

Water Quality Modeling System
for the Great Lakes (WQMSGL)

- Consists of three subsystems that allow user to develop, calibrate, and verify water quality models for aquatic systems
- Developed to serve EPA's research mandates for the Great Lakes, but applicable to any surface water system
- Can be applied to most water quality problems, constituents, and interactions

Holding Office: Office of Environmental Processes and Effects Research
Responsible Person: William Richardson
FTS Phone: 8-226-7811

Unsaturated Zone and Ground Water Fate Models

MINTEQ

- A geochemical model capable of calculating equilibrium aqueous specification, adsorption, gas phase partitioning, solid phase saturation states, and precipitation-dissolution of 11 metals (arsenic, cadmium, chromium, copper, lead, mercury, nickel, selenium, silver, thallium, and zinc)
- Can solve a broad range of chemical equilibrium problems for surface and ground waters
- Contains an extensive thermodynamic data set
- Designed for the DOS environment on the IBM PC XT/AT family of microcomputers and compatible systems
- Language: FORTRAN 77
- Approximate run time using sample data sets: 4 minutes

Contact: Center for Water Quality Modeling
Environmental Research Laboratory
U.S. EPA
Athens, Georgia 30613
404-546-3585

Pesticide Root Zone Model (PRZM)

- Simulates the vertical movement of pesticides in unsaturated soil within and below the plant root zone, and extending to the water table
- Uses generally available input data that are reasonable in spatial and temporal requirements
- Consists of hydrology and chemical transport components that simulate runoff, erosion, plant uptake, leaching, decay, foliar wash-off, and volatilization of a pesticide.
- Designed for the DOS environment on the IBM PC XT/AT family of microcomputers and compatible systems
- Language: FORTRAN 77
- Approximate run time using sample data sets: 8 minutes

Contact: Center for Water Quality Modeling
Environmental Research Laboratory
U.S. EPA
Athens, Georgia 30613
404-546-3585

Pesticides Analytical Transport Solution (PESTAN) or Analytic Transient 1,2,3-Dimensional Model (AT123D)

- Predicts pesticide and organic pollutant movement to ground water
- Environmental and chemical data input interactively
- Available through GEMS
- Version in GEMS features an automated link with Seasonal Soil Model (SESOIL) to allow modeling of chemicals moving from the unsaturated zone into ground water

Holding Office: Office of Environmental Processes and Effects Research
Responsible Person: David M. Walters
FTS Phone: 8-743-2261

Regulator and Treatment Zone Model (RITZ)

- Models pollutant transport by leaching and volatilization
- Estimates biological degradation of the pollutant
- Considers the effect of an oil phase on pollutant transport

Holding Office: Office of Environmental Processes and Effects Research
Responsible Person: Tom Short
FTS Phone: 8-743-2234

Seasonal Soil Compartment Model (SESOIL)

- Long-term fate simulations
- Accounts for numerous hydrologic, meteorologic characteristics of site
- Accounts for numerous transfer, transformation processes: absorption volatilization, degradation, biodegradation
- Models organics, inorganics
- Handles up to three layers of soil types, permeabilities
- Integrated into GEMS
- Versatile, easy to use
- FORTRAN program language; has been implemented on IBM 370, VAX 11/780
- Produces contaminant concentration distribution in unsaturated zone, quality of ground water runoff

Documentation: Bonazountas and Wagner, 1981
Contact for access to GEMS system: Mr. Loren Hall
U.S. EPA, Exposure Evaluation Division
Washington, D.C.
202-382-3931

Simulated Waste Access to Ground Water (SWAG)

- Predicts organic pollutant transport to ground water
- Three compartment analytical computer model
- Considers transformations in the soil-geological matrix
- Data is input interactively by the user

Holding Office: Office of Environmental Processes and Effects Research
Responsible Person: David M. Walters
FTS Phone: 8-743-2261

Three-Dimensional Plumes in Uniform Ground-Water Flow (PLUMEZD)

- Estimates concentration distribution in a leachate plume emanating from a point source
- Includes both linear absorption and first-order reactions

Holding Office: Office of Emergency Processes and Effects Research
Responsible Person: Carl Enfield
FTS Phone: 8-743-2334

Exposure Assessment Models

Mixture and Systemic Toxicant Risk Model (MSRM)

- Estimates human health risk from exposure by any route
- Non-cancer risk assessment models and estimation categories
- Contains statistical methods and extrapolation models for using available toxicological and epidemiological data
- Cancer risk models included for completeness, but developed elsewhere

- Applicable for single chemicals and mixtures
- Estimation methods include those in EPA Risk Assessment Guidelines for Comparison

Holding Office: Office of Health and Environmental Assessment
Responsible Person: Richard Hertzberg
FTS Phone: 8-684-7582

Radionuclide Dose Rate/Risk
(RADRISK)

- Estimates health risk due to inhalation or ingestion of radionuclides for arbitrary exposure periods
- End result in set of values relating fatal cancers and genetically significant radiation doses to a unit of radionuclide intake
- A greatly revised combination of two previously existing programs--INREM II and CAIRD
- Health risk from external expsosure also estimated by CAIRD using dose rates from DOS FACTER

Holding Office: Office of Radiation Programs
Responsible Person: Christopher B. Nelson
FTS Phone: 8-557-9380