# CENTER FOR EXPOSURE ASSESSMENT MODELING

Robert B. Ambrose, Jr., P.E. Manager

Center for Exposure Assessment Modeling Office of Research and Development U.S. Environmental Protection Agency Athens, GA 30613 Center for Exposure Assessment Modeling (CEAM) The Center for Exposure Assessment Modeling (CEAM) was established in July 1987 to meet the scientific and technical exposure assessment needs of EPA's Program and Regional Offices and of State environmental agencies. CEAM is the Agency designated Technical Support Center for Ecological Risk Assessment. The Center is also the focal point for a variety of general Agency support activities related to the scientifically defensible application of state-of-the-art exposure assessment technology for environmental risk-based decisions. CEAM provides exposure assessment technology, training and consultation for analysts and decision-makers operating under various legislative mandates, including FIFRA, CWA, TSCA, RCRA, SDWA, and Superfund.

Distribution   Training   in   Codes and     Model   Applications	Expert   Advice   on   Solving   a   Problem	In-depth Participation in Planning and Conducting Priority Projects
---	--	---

CEAM Offers Direct Support To support the Agency and States in environmental risk-based decisions concerning protection of air, water, and soil, CEAM seeks to expand the expertise of persons who quantitatively evaluate pollutant exposure as part of human and ecological risk assessments.

#### CEAM is organized to:

- o Assist in site-specific problem definition and provide appropriate predictive techniques for accessing organic chemicals and metals exposure through single and multimedia pathways.
- o Maintain the Superfund Ecological Risk Technical Support Center and provide training and assistance to regional and headquarters Superfund staff in exposure and EcoRisk assessments.
- o Maintain a distribution center for continually updated models (codes and documentation) and databases for the user community, including consultants; keep users up to date through user group meetings, a newsletter, and a

computer "bulletin board."

- o Offer 2- to 5-day training sessions at regional sites, headquarters, and the Athens facility using instructors from CEAM, the Center for Environmental Research information, the EPA Training Institute, universities, and consulting firms. Longer term (weeks, months, year) on-the-job training at CEAM for individuals is also available.
- o Provide requested assistance through "expert witness" testimony, exposure calculations and assessments for especially difficult or unusual scenarios, peer review of exposure and EcoRisk assessments, and in-depth support for high priority Agency projects.
- o Assist in conducting exposure and ecological risk assessments for the complete range of EPA needs as part of RCRA, TSCA, FIFRA, and CWA.

CEAM Provides Research Expertise

Exposure assessment expertise is available for multimedia modeling of organic chemical and heavy metal pollutant fate; regional and local air contaminant modeling; source and site characterization, monitoring, and measurement; marine and estuarine pollutant fate modeling; pollutant dose-response modeling; ecological impact and ecological risk assessment. This expertise is drawn from the CEAM and associate staff at the Environmental Research Laboratory, Athens, GA (ERL-Athens), plus experts at affiliated laboratories including the Environmental Research Laboratory, Duluth, MN (ERL-Duluth); the Environmental Monitoring Systems Laboratory, Las Vegas, NV (EMSL-Las Vegas); the Environmental Research Laboratory, Narragansett, RI (ERL-Narragansett); the Atmospheric Sciences Research Laboratory, Research Triangle Park, NC (ASRL); the Environmental Research Laboratory, Gulf Breeze, FL (ERL-Gulf Breeze); the Environmental Monitoring Systems Laboratory, Research Triangle Park, NC (EMSL-RTP); and the Environmental Monitoring and Support Laboratory, Cincinnati, OH (EMSL-Cincinnati).

Multimedia Exposure Assessment--ERL-Athens develops aquatic and terrestrial exposure models and measures or estimates the physical, chemical, and biological properties (rate and equilibrium constants) that are needed for model operation. Environmental decision-making tools include pollutant fate and exposure models; conventional pollutant loading and ecosystem response models; knowledge-based expert systems; multimedia assessment, management, and control strategy development and evaluation methodologies; and procedures for conducting uncertainty analysis. Models are applicable to watersheds, surface and ground waters, agricultural areas, hazardous waste sites, spill sites, water treatment plants.

wildlife habitats, etc.

Air Models--ASRL-RTP conducts research on chemical, physical, and meteorological processes in the environment and develops models to relate pollutant source emissions to air pollutant concentrations at receptor sites and wet- and dry-fall source inputs to land and surface water.

Marine and Estuarine Exposure Models--ERL-Narragansett develops exposure assessment methodologies for quantifying transport and transformation of pollutants in marine and estuarine environments.

Dose-Response Models--ERL-Duluth provides expertise in predicting exposure within and impact on aquatic organisms (dose response), and physiologically based pharmacokinetic models of intoxication processes relating adverse effects on a target organ to the external concentration profile.

Estuarine Effects--ERL-Gulf Breeze provides expertise for predicting the lethal and sublethal impact of exposure to toxic chemicals on pesticides in coastal, estuarine, and marine environments, including effects on individual components and ecological structure and function and the resiliency of populations, communities, and ecosystems.

Monitoring and Measurement Methods--EMSL-Las Vegas designs and conducts remote sensing and field sampling studies and operates monitoring systems to characterize sources and sites for modeling assessment.

Monitoring and Measurement Methods--EMSL-Cincinnati develops analytical methods for the measurement of toxic materials in municipal and industrial wastewaters, ambient waters, solid waste, and Superfund samples.

Air Monitoring--EMSL-RTP develops monitoring systems for measuring air pollutants and determining exposure in ambient air, in indoor air, near toxic waste sites, and conducts special air monitoring studies to assess atmospheric pollution problems and evaluate exposure models.

CEAM Staff

Mr. Robert B. Ambrose, Jr., P.E. - CEAM Manager
404-546-3130
Surface Water Quality
and Pollutant Modeling
Aquatic EcoRisk

Dr. James L. Martin, P.E.

- Environmental
Engineering
Surface Water Quality
and Pollutant Modeling

Mr. Kendall P. Brown

- Chemical Engineering Leaching Modeling Metals Modeling

Mr. David Disney

- Software Systems
Analysis
Model and Documentation
Distribution/Quality
Control.

Mr. Timothy Wool

- Software Systems
Analysis
Water Quality Modeling

### Engineering and Assessment

Dr. David S. Brown

- Metals Modeling Soil Science

Dr. Fred Fong

- Mass Transport Modeling Numerical Analysis and Chemical Engineering

Mr. Thomas O. Barnwell

- Model Applications/ Expert Systems Watershed and Nonpoint Source Modeling

Mr. Robert F. Carsel

- Leaching, Ground Water
Modeling
Environmental
Parameters,
Soil Properties,
Uncertainty Analysis

Dr. Steven C. McCutcheon, P.E.

- Sediment and Pollutant Transport Hydrodynamics

Mr. Lee A. Mulkey

- Multimedia Modeling, Terrestrial Exposure and Risk, Uncertainty Analysis Mr. Charles N. Smith

- Field Sampling and Study Design Model Testing, Monitoring Equipment, Uncertainty Analysis

## Pollutant Identification and Chemical Fate Data

Dr. James J. Ellington

- Hydrolysis Rate
Constants
Partition Coefficients

Mr. Heinz P. Kollig

- Reliability of Fate
Constants in
Literature
Computation of
Unreported
Constants

Dr. John M. McGuire

- Identification of
Transformation
Products and Unknown
Follutants

Dr. William C. Steen

- Biological Transformation Rate Constants

### Chemical and Biological Transformation Processes

Dr. Chad Jafvert

- Sorption Processes

Dr. David L. Lewis

- Biodegradation and Bioaccumulation Processes

Dr. Nicholas Loux

- Metals Speciation and Sorption to Aquifer Surfaces

Dr. John E. Rogers

- Anaerobic Biotransformation Processes Dr. Eric Weber

- Chemical Properties,
Degradation Rates and
Products of Organic
Pollutants

Dr. N. Lee Wolfe

- Hydrolysis and Reduction Processes

Dr. Richard G. Zepp

- Organic Photolysis and Oxidation Processes

Ecological Risk Assessment

Dr. Lawrence A. Burns

- Wetlands Ecology

Dr. James Hill

- Aquatic Food Chain Exposure Models Ecological Risk Assessment

Dr. Ray R. Lassiter

- Ecological Risk
Assessment Modeling

CEAM Models Meet Analysts' Needs The modeling packages currently available through CEAM were selected from many candidate models by experienced users in EPA regulatory and regional offices and by the Center staff. Selection criteria included model utility and effectiveness, availability of adequate documentation, degree of acceptance and application by users, and the Center staff's experience with the model. A wide range of analysis techniques is provided, from simple desk-top procedures suitable for screening analysis through computerized steady-state models to sophisticated, state-of-the-art continuous simulation models. Supported models are available for microcomputer and mainframe system applications.

WQA

A collection of formulas, tables, and graphs allows planners to make preliminary assessments of surface and ground water quality in large river basins. These desk-top procedures are appropriate for hand calculators. The manual includes a discussion of the environmental chemistry of synthetic organic chemicals and metals; a chapter on waste source estimation techniques; and simple methods for assessment of pollutant fate in rivers, lakes, estuaries and ground water.

Stream analysis techniques are included for conservative substances, water temperature, biochemical oxygen demand, dissolved oxygen, total suspended solids, coliform bacteria, nutrients, and toxic organic chemicals and metals. Lake analysis procedures include thermal stratification, sediment accumulation, toxic organic chemicals, phosphorus budget, eutrophication potential, and hypolimnion dissolved oxygen. Estuarine analyses include estuarine classification, temperature, biochemical oxygen demand, dissolved oxygen, turbidity, sediment accumulation, and non-conservative substances.

Ground water procedures include aquifer characterization, the ground water flow regime, pollutant transport processes, methods for predicting the fate and transport of conventional and toxic pollutants, and interpretation of results. Documentation: Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants in Surface and Ground Waters. EPA/600/6-85/002a-c.

QUAL2E

Conventional pollutants in one-dimensional streams and well-mixed lakes all modeled under steady state conditions. The conventional pollutants include conservative substances, temperature, bacteria, biochemical oxygen demand, dissolved oxygen, nitrogen, phosphorus, and algae. QUAL2E is widely used for waste load allocations and discharge permit determinations in the United States and other countries. It has a 15-year history of application and is a proven, effective analysis tool. QUAL2E Version 3 incorporates several uncertainty analysis techniques useful in risk assessment. Documentation: The Enhanced Stream Water Quality Models QUAL2E and QUAL2E-UNCAS. EPA/600/3-87/007. (4 diskettes)s

DYNTOX

A waste load allocation computer program uses a probabilistic dilution technique to estimate concentrations of toxic substances or fractions of whole effluent toxicity. DYNTOX performs three types of simulations -- continuous, monte carlo, and log normal -- that, based on probabilities, can aid in analyzing the frequency and duration of toxic concentrations from a waste discharge. DYNTOX considers dilution and net first-order loss, but not sorption and benthic exchange. The net loss rate must be determined on a case-by-case basis and should not be extrapolated to different conditions of flow, temperature, solids, pH, or light. Documentation: Dynamic Toxics Wasteload Allocation Model (DYNTOX). (3 diskettes)

MINTEQA1

A geochemical model calculates equilibrium aqueous speciation, 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). MINTEQAl contains an extensive thermodynamic data base and six

different algorithms for calculating adsorption. Proper application of MINTEQA1 requires user expertise, because kinetic limitations at particular sites may prevent certain reactions even though they might be thermodynamically possible. (5 diskettes)

Documentation: MINTEQA1, An Equiblibrium Metal Speciation Model. EPA/600/3-87/012.

#### EXAMS-II

A steady-state and dynamic model rapidly evaluates the behavior of synthetic organic chemicals in lakes, rivers, and estuaries. EXAMS-II is an interactive program that allows the user to specify and store the properties of chemicals and ecosystems, modify the characteristics of either (via simple English-like commands), and conduct rapid, efficient evaluations of the probable fate of chemicals. EXAMS-II simulates a toxic chemical and its transformation products using second-order kinetics for all significant organic chemical reactions. EXAMS-II, however, does not simulate the solids with which the chemical interacts. The concentration of solids must be specified for each compartment; the model accounts for sorbed chemical transport based on solids concentrations and specified transport fields. Benthic exchange includes pore water advection, pore water diffusion, and solids mixing. The latter describes a net steady-state exchange associated with solids that is proportional to pore water diffusion. (4 diskettes) Documentation: Exposure Analysis Modeling System (EXAMS-II).

EPA/600/3-85/038.

SWMM

Urban runoff quantity and quality is comprehensively simulated. All aspects of the urban hydrologic and quality cycles are simulated including surface runoff, transport through the drainage network, and storage and treatment (including cost). Alternate techniques are available for simulation in a sewer system -- a kinematic wave procedure for most problem assessment and a full-equation routing method for surcharged systems. SWMM can be used both for singleevent and for continuous simulation. It has been used in a planning context as well as for detailed design studies. SWMM also has a long history of use for urban drainage assessment and design. (4 diskettes) Documentation: Storm Water Management Model, Version 4. EPA/600/3-88/001.

HSPF

Watershed hydrology and water quality for both conventional and toxic organic pollutants is simulated. HSPF incorporates the watershed-scale ARM (Agricultural Runoff Model) and NPS (Non-Point Source) models into a basin-scale analysis framework that includes pollutant transport and transformation in stream channels.

The model uses information such as the time history of rainfall, temperature, and solar radiation; land surface

characteristics such as land use patterns and soil properties; and land management practices to simulate the processes that occur in a watershed. The result of this simulation is a time history of the quantity and quality of runoff from an urban or agricultural watershed. Flow rate, sediment load, and nutrient and pesticide concentrations are predicted. The program takes these results, along with information about the stream network and point source discharges, and simulates instream processes to produce a time history of water quantity and quality at any point in a watershed -- the inflow to a lake, for example. HSPF includes an internal data base management system to process the large amounts of simulation input and output. (6 diskettes) Documentation: Hydrological Simulation Program--FORTRAN. EPA/600/3-84/066.

PRZM

The vertical movement of pesticides in unsaturated soil, both within and below the plant root zone, and extending to the water table using generally available input data that are reasonable in spatial and temporal requirements. The model consists of hydrology and chemical transport components that simulate runoff, erosion, plant uptake, leaching, decay, foliar wash off, and volatilization (implicitly) of a pesticide. Predictions can be made daily, monthly, or annually. Documentation: User's Manual for the Pesticide Root Zone Model (PRZM). EPA/600/3-84/109 (2 diskettes)

WASP

A generalized modeling framework simulates contaminant fate and transport in surface waters. Based on the flexible compartment modeling approach, WASP can be applied in one, two, or three dimensions. WASP is designed to permit easy substitution of user-written routines into the program structure. Problems that have been studied using WASP include biochemical oxygen demand, dissolved oxygen dynamics, nutrients and eutrophication, bacterial contamination, and toxic chemical movement.

A variety of water quality problems can be addressed with the selection of appropriate kinetic subroutines that may be either selected from a library or written by the user. Toxics WASF combines a kinetic structure adapted from EXAMS with the WASP transport structure and simple sediment balance algorithms to predict dissolved and sorbed chemical concentrations in the bed and overlying waters.

Eutrophication WASP combines a kinetic structure adapted from the Potomac Eutrophication Model with the WASP transport structure. EUTRO4 predicts dissolved oxygen, carbonaceous biochemical oxygen demand, phytoplankton, carbon, and chlorophyll a, ammonia, nitrate, organic nitrogen, and orthophosphate in the bed and overlying waters. (3 diskettes) Documentation: WASP4, a Hydrodynamic Water Quality Model for Toxic and Conventional Pollutants. EPA/600/3-87/039.

DYNHYD4

A simple link-node hydrodynamic model simulates variable tidal cycles, wind, and unsteady inflows. It produces an output file that can be linked with WASP4 to supply the flows and volumes to the water quality model.

The Food Chain Model is an associated program that takes the time and space-variable pollutant concentrations calculated from WASP4, and predicts uptake and distribution throughout a user-described aquatic food chain. (w/WASP) Documentation: WASP4, a Hydrodynamic Water Quality Model for Toxic and Conventional Pollutants. EPA/600/3-87/039.

SARAH

A steady-state mixing zone model calculates acceptable concentrations of hazardous wastes discharged to land disposal or waste water treatment facilities. For steady or batch waste streams. SARAH considers the following concentration reductions: dilution and loss during treatment, initial Gaussian mixing at the edge of a stream, lateral and longitudinal diffusion in the mixing zone, sorption, volatilization, Hydrolysis, and Bioaccumulation in fish. The user must specify appropriate in-stream criteria for protection of the aquatic community, and of humans through consumption of fish and water. The benthic community is not presently considered. Treatment loss is handled empirically. The human exposure pathways considered include ingestion of treated drinking water and consumption of contaminated fish. Documentation: SARAH, a Surface Water Assessment Model for Back-calculating Reductions in Abiotic Hazardous Wastes. EPA/600/3-86/058. (1 diskette))

FGETS

A toxicokinetic model simulates the bioaccumulation of nonpolar organic chemicals by fish from both water and tainted food. Both of these routes of exchange are modeled as diffusion processes that depend upon physico-chemical properties of the pollutant and morphological/physiological characteristics of the fish. FGETS contains a moderately sized database of allometric relationships for gill morphology with which it can simulate the direct gill/water exchange of organic chemicals for essentially any fish species, assuming certain default values. FGETS also contains a limited database of physiological/morphological relationships that are used to parameterize food exchange. Presently, only food exchange by salmonids is represented in the database. However, this database is being expanded to centrarchids, perchids, and cyprinids. In addition to simulating bioaccumulation of organic toxicants, FGETS can also calculate time to death from chemicals whose mode of action is narcosis. This calculation is based on the existence of a single, lethal, internal chemical activity for such chemicals. (1 diskette) Documentation: FGETS (Food and Gill Exchange of Toxic Sub-

Documentation: FGETS (Food and Gill Exchange of Toxic Substances): A Simulation Model for Predicting Bioaccumulation of Nonpolar Organic Pollutants by Fish. EPA/600/3-87/038.

Models in Development

Several model development projects are underway to provide additional modeling tools to support Agency regulatory programs. The research and development programs producing these models at the ERL-Athens include projects on ecological risk assessment, land disposal of hazardous wastes, and exposure assessment models for pesticides.

Multimedia Exposure Assessment Model for Hazardous Wastes simulates the release and fate of hazardous waste constituents derived from land disposal systems. Soil (unsaturated zones), atmospheric, ground water, and surface water routes are included. The model is implemented within a monte carlo framework to facilitate uncertainty analysis as an integral part of risk assessment.

Pesticide Ground Water Exposure Assessment Model provides a linked system of models that combines root zone dynamics (PRZM) with unsaturated-saturated zone transport and transformation predictions for pesticides. The modeling package combines one- and two-dimensional finite element codes and enables simulation of a wide range of environmental settings. This model is also implemented within a monte carlo framework to facilitate uncertainty analysis.

Terrestrial Environmental Exposure Assessment Model computes the distribution, movement, and potential ecological impact of chemical pollutants released to terrestrial environments. Atmospheric transport and interactions within the soil-plant-water complex are included.

Drinking Water Treatment Plants can be simulated by combining the unit operations typically employed in designed systems. This model uses chemical-specific data and mass transport theory to estimate the exposure reductions achieved by treating contaminated drinking water. Model capability ranges from simple operations typical of small, rural water supply systems to large-scale municipal systems.

CEAM Services Are Readily Obtained The Center also functions as a clearinghouse for correcting code and routine errors or other problems that are discovered as the techniques are applied. This vital information exchange function helps users obtain correct computations when applying a model developed for one purpose to a new and different problem. New software releases periodically document code updates and corrections to problems identified as the models are used. Model maintenance activities focus on overcoming problems in the use of models; further development, refinement, and extension of these models is a separate research activity.

The Center periodically distributes, free of charge, a newsletter to a large number of model users and developers in the Agency, other federal, regional and state environmental management agencies and their consultants, international agencies, and private industry and academia. The newsletter provides helpful hints to model users and communicates information on scheduled workshops, model improvements and developments, the availability of technical documents, and planned meetings and conferences.

Consultation

For consultation or technical assistance on exposure or EcoRisk assessment projects, write or call the CEAM manager,

Mr. Robert B. Ambrose, Jr.
CEAM
US E.P.A.
College Station Road
Athens, Georgia 30613

(404) 546-3130 or FTS 250-3130

For information about or assistance with CEAM models, write to CEAM model support at the above address or call the CEAM model support line at (404) 546-3549 or FTS 250-3549. You may also correspond with us by using the CEAM electronic bulletin board system as described below.

PC and Mainframe Models The models are available from the CEAM at no charge. Mainframe versions of the programs compatible with DEC VAX systems are available on standard one-half inch, 9-track magnetic tape. When ordering tapes, please specify the type of computer system that the model will be installed on (VAX, PRIME, HF, CYBER, IBM, etc.) and whether the tape should be non-labeled. If non-labeled, specify the storage format as ASCII or EBCDIC. If the tape is for a DEC system, specify the storage format as VAX Files-11 (ASCII). Requests for PC versions of the models should be accompanied by the appropriate number of double-sided, double-density (DS-DD), errorfree diskettes. To obtain copies of the models, please send 9-track specifications, or the appropriate number of diskettes, to the attention of David Disney at the Center for Exposure Assessment Modeling. Program and/or user documentation, or instructions on how to order documentation, will accompany each response, in addition to installation instrucitons.

Electronic Bulletin Board The CEAM Electronic Bulletin Board Systems (BBS) is designed to meet the increasing demand for exposure assessment models supported by the Center. It provides more efficient communication between users and support staff, as well as immediate acquisition of models by those users under extreme time pressure. The CEAM BBS has been installed using a commercially available software package. The BBS is available days a week, 24 hours a day. The System Operator may be paged through the BBS from 7:00 a.m. until 4:00 p.m. Monday thru Friday for assistance.

The services presently offered through the BBS are: 1. down-loading of CEAM-supported simulation models; 2. Uploading of user input data sets for staff review and problem solving; 3. listing of current activities and events, (such as training courses) helpful hints about the models, and model documentation; and 4. message area for discussion of computer modeling problems and enhancements.

To access the CEAM BBS, call 404/546-3402 or FTS/250-3402 and follow the interactive prompts. The communications parameters needed are 2400/1200 baud, no parity, 8 data bits, and 1 stop bit. To access the CEAM BBS via the EPA Dec Net, type SET HOST ATHENS, USERNAME=BBS, PASSWORD=ATHENS. This will allow access to the CEAM BBS without long distance charges. Downloading of models and uploading of datasets is not possible through Dec Net; however, the user will be able to access the bulletin area and leave and/or read BBS messages.