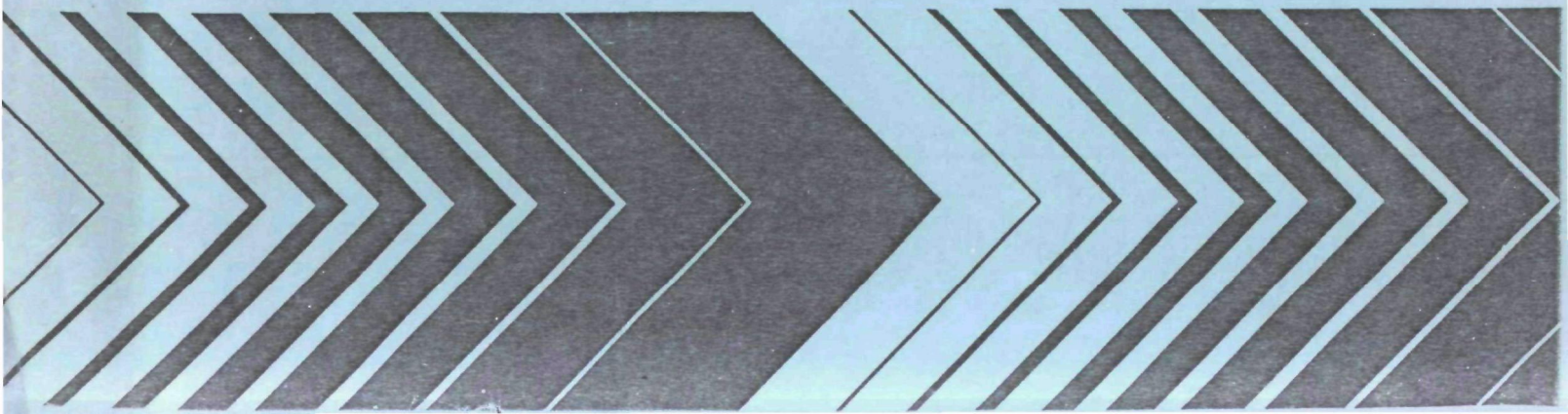




Research Report

**Environmental
Research
Laboratory
Athens, GA 30613**



THIRD QUARTER STATUS REPORT ON FY87 PROJECT DESCRIPTIONS

This report summarizes Athens Environmental Research Laboratory research activities for the period April 1, 1987 to June 30, 1987.

The status of work in progress toward meeting major planned outputs is presented under descriptive project titles. The report is an interim summary of ongoing research with tentative conclusions based on careful analysis of the research findings to date. Project managers identified with each activity would be pleased to provide additional information.

Highlights

Data Generated for Risk Assessment Models--Athens Laboratory chemists recently have developed hydrolysis rate constants for 54 organic chemicals and octanol-water partition coefficients for an additional 22 chemicals. The work is part of a continuing project to develop input data for models for assessing risk to human health posed by land disposal of hazardous waste. In the project for the Office of Solid Waste, 85 hydrolysis rate constants and 40 partition coefficients have now been measured or obtained from the literature. Dr. Jackson Ellington, Mr. Frank Stancil, Mr. Bill Payne, and Ms. Cheryl Trusty are now working on the "third-third" of the list of 362 compounds provided by OSW.

Updated QUAL2E Published--Printed copies of The Enhanced Stream Quality Models QUAL2E and QUAL2E-UNCAS (EPA/600/3-87/007) are now available. The documentation, prepared by Dr. Lin Brown of Tufts University and Mr. Tom Barnwell of the Athens Lab, presents the revised QUAL2E model, which is widely used for discharge permit determinations, waste load allocations, and other conventional pollutant evaluations. The model is enhanced by an uncertainty analysis component. This enhancement allows the user to conduct sensitivity analysis, first order error analysis, and monte carlo simulation.

Athens Lab-Duluth Lab Paper Published--"Toward Modeling the Effects of Chemicals Acting Jointly," a paper coauthored by Dr. Ray Lassiter of ERL-Athens and by Dr. Steven Broderius of ERL-Duluth has been published in Methods for Assessing the Effects of Mixtures of Chemicals. The paper describes a model developed to account for exchange of chemicals between the external aqueous medium and an organism's body. Based on the model, the relative times required for different chemicals to reach a steady state in the body relative to external concentrations is found to be in direct proportion to the ratio of their octanol-water partition coefficients.

This document has not been peer and administratively reviewed within EPA and is for internal Agency use/distribution only.

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THIRD QUARTER STATUS REPORT ON FY'87 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

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CODE      TITLE
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BUDGET SUB-ACTIVITY: B101  WATER
ISSUE: A      WQBA/PERMITTING
PPA (L): 10    WASTELOAD ALLOCATION MODELING AND SUPPORT
PPA (S): 10    WASTELOAD ALLOCATION
RC: K          ERL ATHNS
PROJECT: 06     Environmental Process Characterization
PROJECT OFFICER: Richard G. Zepp      PHONE: FTS-250-3428
*****
PLANNED START: 10/01/80    PLANNED END: 09/30/90
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PROJECT DESCRIPTION:

GOAL: Characterize key environmental processes (direct-indirect photolysis, redox, sorption/desorption, metal binding) in water and sediment systems to improve exposure and risk assessment models.

RATIONALE: The roles of inorganics in pollutant transformation by photolysis and the kinetics of redox reactions are inadequately understood for reliable use in exposure assessment models. These processes are known to be environmentally important in many cases. Toxic metal speciation and transport needs further investigation since metal toxicity depends upon the species involved.

APPROACH: Laboratory studies using natural waters, sediments and reference materials will be conducted to test proposed equations for the kinetics of transformation processes. The studies will provide rate/equilibrium constants required in the models. Compounds and reaction conditions will be selected to permit generalizations about changes in molecular structure and environmental occurring inorganic species; redox reactions of abiotic systems will be studied relative to biotic influences. The binding characteristics of metals with humic materials will be studied and distribution coefficients determined.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The interactions of photochemically produced iron(II) with hydrogen peroxide and resulting organic oxidations were studied during the quarter. Using anisole and nitrobenzene as chemical probes and octanol or formate ion as scavengers, we found that the yield of hydroxyl radicals from Fe(II)/hydrogen peroxide was 40% at pH 6.2. A promising technique was developed for the direct simultaneous analysis of Fe(III) and Fe(II) in natural waters. Dr. Richard Zep is stationed for the summer at the EAWAG Laboratory in Switzerland, studying photochemical processes with Swiss scientists.

Nitrobenzene reduction studies were extended to soil-water samples obtained from two aquifers. The disappearance rate constants were approximately five

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ERL ATHNS: APRIL - JUNE 1987

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

times slower in the aquifer samples than in sediment samples collected in the Athens area. Detailed concentration studies of substituted nitrobenzenes indicated that the disappearance rate constants were dependent on the initial concentration of the nitrobenzene derivative. Additional studies are in progress to determine the rate limiting step of the reduction process.

Redox studies were performed on two carbamate pesticides, Protham and Carbaryl, in an anaerobic sediment/water system containing 10% solids. Kinetic results are being interpreted; decay products of these two pesticides will be analyzed. In addition to these redox studies, the hydrolysis of chlorinated organic compounds is currently being investigated.

Studies of the degradation of synthetic dyestuffs in anaerobic sediments continue. The effects of pH on the distribution and kinetics of reduction were studied for a nonionizable dye, azobenzene, and an ionizable dye, Congo Red. Results indicate that pH will have little effect on the distribution and reduction of azo dyes containing non-ionizable functional groups. For those dyes that do contain ionizable groups, pH will play an important role in their distribution and, thus, transport in natural systems. Changes in pH, however, may have little effect on the rate of reduction of these dyes at the sediment-water surface.

Studies on sorption of ionizable organic compounds to soils, sediments and aquifer material continue. Experimental work confirms that partitioning of the anion of pentachlorophenol (pentachlorophenolate) between octanol and water is highly dependent on ionic strength of the water phase and that partitioning if both the ion-paired phenolate and free phenolate species into octanol is important.

A workshop entitled "Oxidation-Reduction Processes in Sediment/Water/Aquifer Systems" was sponsored by ERL-Athens at Estes Park, CO, April 28-30, 1987. A workshop on the Environmental Chemistry of Dyes, organized by the Athens Laboratory, has been tentatively scheduled for November 12-13, 1987, in Pensacola, FL. A symposium entitled "Environmental Chemistry of Ionic Xenobiotics," also organized by the Athens Laboratory, will be held at the SETA Conference in November.

A reverse osmosis sampling system was developed, tested, and used on-site by Georgia Institute of Technology personnel to collect and concentrate by twenty-fold 200g of dissolved organics in Suwannee River (Okefenokee Swamp) water. Ninety-five percent recovery of total dissolved organics was obtained. This organic material will be fractionated to provide the necessary quantity of fulvic and humic acids for use by Georgia Tech, University of Georgia, and inhouse researchers studying metal-organic interactions.

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Work continues at the University of Georgia on use of laser-excited lanthanide ion fluorescence for characterization of metal binding sites in humic materials. Several experiments were completed to establish the precision and accuracy of the recently installed spectrometer system. These included experimental measurement of the emission spectra and lifetimes of Eu(III). Most importantly, confirmation of earlier experimental results on the binding of Eu(III) by humic acid was attained.

SCHEDULE AND STATUS OF DELIVERABLES:

7153 JOURNAL ARTICLE ON INDIRECT PHOTOCHEMICAL PROCESSES IN AQUATIC ENVIRONMENTS.
DUE: 12/31/86 REVISED: 01/01/00 COMPLETED: 12/31/86

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THIRD QUARTER STATUS REPORT ON FY'87 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

CODE	TITLE
BUDGET SUB-ACTIVITY: B101	WATER
ISSUE: A	WQBA/PERMITTING
PPA (L): 10	WASTELOAD ALLOCATION MODELING AND SUPPORT
PPA (S): 10	WASTELOAD ALLOCATION
RC: K	ERL ATHNS
PROJECT: 11	Biodegradation & Bioaccumulation Processes and Systems Res.
PROJECT OFFICER: David L. Lewis	PHONE: FTS-250-3358

PLANNED START: 10/01/85	PLANNED END: 09/30/95

PROJECT DESCRIPTION:

GOAL: To test the predictive accuracy and determine the applicability of microbial transformation rate coefficients for water quality models and to evaluate bioaccumulation of toxicants in aquatic organisms in relation to thermodynamic equilibrium processes.
RATIONALE: This research is required to produce a reliable approach to predicting biologically mediated accumulation and degradation of pollutants for water quality and risk assessment models.
APPROACH: Rate coefficients for microbial transformation of xenobiotic chemicals will be determined using microbial populations collected from fresh water field sites. Bioaccumulation in organisms of varying size, lipid content and species will be determined using toxic chemicals with varying partition coefficients. Coefficients determined in the laboratory will be compared with field data. Predictions based on thermodynamic calculations will be compared with experimental results.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A paper, "Predicting Substrate Removal Rates of Attached Microorganisms and the Relative Contributions of Attached and Suspended Communities in the Field" (Lewis and Gattie) was submitted to Applied and Environmental Microbiology. An abstract, "Predicting Substrate Removal Rates and the Relative Contributions of Attached and Suspended Microbial Communities in the Field" (Lewis and Gattie), has been cleared for a poster presentation at the 1987 SETAC meeting in Pensacola, FL. Also, one paper, "Microbial Biogeochemical Processes in a Naturally Acidic Wetland, the Okefenokee Swamp" (Hodson, Moran, Lewis, Murray, Teska, and Benner), is being cleared for publication in the CRC series, "Microbial Interactions in Acid Stressed Aquatic Ecosystems" (S.S. Rao, ed.).

Field studies using two esters of 2,4-dichlorophenoxyacetic acid and diethyl phthalate are being conducted to evaluate the usefulness of a second-order model for predicting degradation rates of organic substrates by attached

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

microbiota. The model is applicable to shallow aquatic ecosystems such as streams and wetlands.

A complete set of lipid fractions standards has been run on the Iatroscan thin-layer chromatography instrument, and the curves analyzed by Labtech Chrom. Characterization and quantification of fish lipids can now be carried out for use in the development of models for exchange of neutral organics.

SCHEDULE AND STATUS OF DELIVERABLES:

- # 6881 Report on the Relationship Between Lipid Content, Body Burden, and Thermodynamic Calculation of Bioaccumulation
DUE: 07/31/86 REVISED: 07/31/87 COMPLETED: 07/31/87
- # 7671 JOURN. ART. ON PREDICTING SUBSTRATE REMOVAL RATES OF ATTACHED MICROORGANISMS & THE RELATIVE CONTRIBUTIONS OF ATTACH. & SUSPENDED COMMUNITIES IN THE FIELD
DUE: 08/30/88 REVISED: 01/01/90 COMPLETED: 01/01/90

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

	CODE	TITLE
BUDGET SUB-ACTIVITY:	B101	WATER
ISSUE:	A	WQBA/PERMITTING
PPA (L):	10	WASTELoad ALLOCATION MODELING AND SUPPORT
PPA (S):	10	WASTELoad ALLOCATION
RC:	K	ERL ATHNS
PROJECT:	19	Wasteload Allocation Modeling and Support
PROJECT OFFICER:	Robert B. Ambrose	PHONE: FTS-250-3546
PLANNED START:	10/01/80	PLANNED END: 12/31/99

PROJECT DESCRIPTION:

GOAL: Assemble, modify or develop, and test arrays of wasteload allocation (WLA) models for conventional and toxic pollutants for streams, rivers, lakes, and estuaries and provide OW with guidance and user assistance through the Center for Water Quality Modeling (CWQM).

RATIONALE: Water quality-based NPDES revisions, WLAs, AWT assessments, use-attainability activities, and BMP selection by CW, Regions, States, and local governments require scientifically defensible modeling packages including documentation, data bases, training, and user assistance.

APPROACH: Gaps in existing WQ modeling packages will be identified through applied studies conducted in cooperation with OW and with ORD Laboratories. Developments or modifications will fill scientific gaps (e.g., metals speciation and sediment-water pollutant exchange routines) and improve ease-of-use (e.g., interactive model setups and microcomputer packages). User assistance will include developing guidance documents, operating the CWQM to training seminars and workshops as required, and providing hands-on users on request as resources permit.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Test versions of the WASP4.1 program, generalized from WASP3, WASTOX, and EXAMSII, are ready for distribution to peer reviewers. An HSPF PC-compatible release was completed. The PC version is a full implementation of the HSPF program. Comparisons between IBM PC/AT and DEC VAX indicate PC performance is only 6 to 8 times slower than the VAX's optimum performance.

Tom Barnwell, Scarlett Vandergrift, and John Connolly presented a workshop on the Water Analysis Simulation Program (WASP) in Madrid, Spain, May 15-22, 1987.

A paper, "Water Quality Software Available from U.S. EPA" (7152C), by Tom Barnwell, Bob Ambrose, and Scarlett Vandergrift was published in the Interna-

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

tional Association on Water Pollution Research and Control (IAWPRC) newsletter.

Dr. Steve McCutcheon attended a meeting of the Green Bay Modeling Committee to assist Great Lakes National Program Office and ERL-Duluth in design of studies of Green Bay, May 27-28, 1987.

The Center for Water Quality Modeling distributed 602 PC versions of supported models during the second quarter of FY87.

SARAH was refined for implementation on microcomputer. All current scenarios have been completed and tested. Scenarios for oily wastes will be added later.

SCHEDULE AND STATUS OF DELIVERABLES:

- # 7158 REPORT ON UPDATED DOCUMENTATION FOR QUAL II INCLUDING UNCERTAINTY ANALYSIS.
DUE: 09/30/86 REVISED: 02/28/87 COMPLETED: 02/28/87
- # 7551 ONE EXISTING TRAINING COURSE THROUGH CWQM
DUE: 09/30/87 REVISED: 09/30/88 COMPLETED: 01/01/90
- # 7552 TWO NEW TRAINING COURSES THROUGH CWQM, POSSIBLY INCLUDING MINTEQ, EXAMS II AND DYNTOX. (K)
DUE: 09/30/87 REVISED: 01/01/90 COMPLETED: 01/01/90

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

CODE	TITLE
BUDGET SUB-ACTIVITY: B101	WATER
ISSUE: A	WQBA/PERMITTING
PPA (L): 13	ECOLOGICAL RESEARCH WITH THE PEOPLE'S REPUBLIC OF CHINA
PPA (S): 13	CHINA AGREEMENT - WQ
RC: K	ERL ATHNS
PROJECT: 20	Ecological Research with the Peoples Republic of China (PRC)
PROJECT OFFICER: Rosemarie C. Russo	PHONE: FTS-250-3134

PLANNED START: 10/01/84	PLANNED END: 09/30/89

PROJECT DESCRIPTION:

GOAL: Participate jointly with PRC scientists and engineers in the refinement, application and field testing of environmental fate and exposure models for pollution control strategy development and assessment and in the study of environmental transformation processes.

RATIONALE: To support U.S. policy to provide scientific and technological cooperation with the PRC, specifically Annex 3 of the 1980 US-PRC Environmental Protection Protocol.

APPROACH: Via a combination of tailored model refinement projects and technology transfer workshops, the PRC will be helped to acquire and apply an array of appropriate environmental assessment methodologies for their use. Athens ERL will design and monitor PRC field evaluations of selected models. The technology developed and transferred will also be high priority for region/state use in the U.S. Metals process characterization studies will also be conducted to elucidate the transformation and transport of metals in surface and subsurface environments.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Mr. Jin of Chinese Research Academy of Environmental Sciences (CRAES) is working at ERL-Athens on metal interactions with humic substances. The absorption spectra of well-characterized humic substances were recorded with the scattered transmission accessory at different pH levels and saturated with different metal cations. This approach resulted in the resolution of bands not reported previously; the location and intensity of the absorption bands varied with pH and character of the metal cation. Analysis of these bands is expected to provide clues to the nature of the metal binding chromophores. Sorption studies of 14 metals with humic substances at pH 4 were completed and the resulting isotherms calculated. Competitive sorption (14 metals of equal concentration) studies with different humic substances were completed.

Mr. Lin of Beijing University is working at ERL-Athens on metal inter-

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ERL ATHNS: APRIL - JUNE 1987

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

actions with sulfides. Four sulfide minerals--pyrite, galena, chalcocite and sphalerite--were selected and size fractions obtained. Removal of sulfur oxidation products on the pyrite surface was necessary prior to any sorption studies. Sorption studies of 10 metals singularly with the four sulfide minerals and competitive sorption with 10 metals were completed; suspension pH was that of the mineral suspension. Adsorption isotherms, partition coefficients and thermodynamic parameters are being calculated.

Robert Ambrose, Steven McCutcheon, and Mac Long conducted a WASP4 workshop in Beijing for Chinese scientists from collaborating institutes. This model will be used in collaborative US-PRC studies. Detailed research plans are being developed for the Lake Beston study (Xinjiang Institute) and Harbor Study (Nanjing University).

The joint US-PRC-Canada Symposium on Fish Physiology, Toxicology, and Management is now scheduled for September 14-16, 1988, in Guangzhou.

Source Code and Example Applications for QUAL2E Version 3.0 were prepared for release in July.

PRC visiting research associate, Mr. Qian Song, has produced interesting results exploring the impact of covariance among model inputs on uncertainty analysis. Using O'Connor's analytical solution to the Streeter-Phelps equation, he found that consideration of covariance results in a 23-30% increase in uncertainty estimates. These results, if confirmed, are significant as they indicate that we cannot make the assumption of independence in model inputs.

SCHEDULE AND STATUS OF DELIVERABLES:

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|--------|---------------------------------------------------------------------------------------------------------------------------|-------------------|---------------------|
| # 7174 | MAGNETIC TAPE OF SWMM III.4 INCLUDING CORRECTIONS AND ENHANCEMENTS
DUE: 12/31/87 | REVISED: 01/01/00 | COMPLETED: 01/01/00 |
| # 7556 | INTERNAL REPORT ON APPLICATION OF MODELS FOR CONVENTIONAL AND TOXIC POLLUTION ASSESSMENT IN THE PRC. (K)
DUE: 09/30/87 | REVISED: 01/01/00 | COMPLETED: 01/01/00 |
| # 7557 | INTERNAL REPORT ON JOINT US-PRC STUDIES ON POLLUTANT TRANSFORMATION PROCESSES. (K)
DUE: 09/30/87 | REVISED: 01/01/00 | COMPLETED: 01/01/00 |
| # 7673 | REPORT ON MODIFICATION/APPLICATION OF QUALII E-UNCAS FOR WASTELOAD ALLOCATION. (K)
DUE: 11/30/87 | REVISED: 01/01/00 | COMPLETED: 01/01/00 |

THIRD QUARTER STATUS REPORT ON FY'87 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

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***** ERLATHNS:APK1L JUNE 1987 *****
CODE      TITLE
BUDGET SUB-ACTIVITY: B101  WATER
ISSUE: A    WQBA/PERMITTING
PPA (L): 15  ARTIFICIAL INTELLIGENCE AND EXPERT SYSTEMS
PPA (S): 15  EXPERT SYSTEMS
RC: K        ERLATHNS
PROJECT: 08   Expert System for Prediction of Physical/Chemical Parameters
PROJECT OFFICER: Samuel W. Karickhoff      PHONE: FTSJ250-3149
*****
***** PLANNED START: 06/01/85    PLANNED END: 09/30/88 *****
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PROJECT DESCRIPTION:

GOAL: To develop computational methods for estimation of fundamental reactivity parameters (rate constants, equilibrium constants, etc.) for various compounds based on their molecular structures alone.

RATIONALE: A major portion of the pollutant fate program at Athens ERL is devoted to the mathematical relationships describing the rate/extent of individual transformation/transport pathways for pollutants in aquatic or terrestrial ecosystems. Current models require as inputs certain fundamental reactivity parameters. Algorithms providing for a priori estimation of these chemical parameters are needed to enable use of process models in situations where measured parameters are not available. Recent advances in computer technology enable the use of computers to integrate theoretical (qualitative and quantitative) and heuristic reasoning with appropriate data to produce predictive algorithms of the type needed.

APPROACH: An expert systems shell will be constructed to: (1) discriminate noncontributing units, (2) develop rules for classifying and characterizing users calibrate with regard to reactivity.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Approximately 15,000 ionization constants for pK_a and pK_b have been collected from the literature and cataloged. A pK database has been designed for input of the constants. This will be used to test the reliability of the computational algorithm for predicting values of pK_a and pK_b . The algorithm for computing pK has been written in Prolog.

An additional 580 UV absorption spectra have been digitized and added to the spectral database. This database will be used for calibration of computational algorithms and validation of the expert system's predictive capability for photochemical rate constants. The scheme for computing steric effects of substituent groups at two levels distant from the center of mass of the molecule was implemented.

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 ERL ATHNS: APRIL - JUNE 1987

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Work continues to: 1) develop a second molecular orbital computational scheme suited for non-alternate organic compounds, 2) extend structural query and spectral computational schemes to compounds having three or four condensed rings, and 3) evaluate software and modify the code for graphic input of molecular structure into SPARC.

SCHEDULE AND STATUS OF DELIVERABLES:

6927 Journal Article Describing Algorithms for Estimating
 Photochemical Rate Constants from Chemical Properties
 DUE: 01/31/87 REVISED: 01/01/90 COMPLETED: 01/31/87

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 ERL ATHNS: APRIL - JUNE 1987

CODE	TITLE
BUDGET SUB-ACTIVITY: B101	WATER
ISSUE: A	WQBA/PERMITTING
PPA (L): 15	ARTIFICIAL INTELLIGENCE AND EXPERT SYSTEMS
PPA (S): 15	EXPERT SYSTEMS
RC: K	ERL ATHNS
PROJECT: 18	AI/ES for Environmental Management
PROJECT OFFICER: Thomas Barnwell	PHONE: FTS-250-3175

PLANNED START: 10/01/85	PLANNED END: 12/31/90

PROJECT DESCRIPTION:

GOAL: To develop, modify and apply experimental knowledge-based expert systems for environmental assessment needs.
 RATIONALE: Use of expert systems (ES) in model calibration, application, and verification will provide uniformity of model application for NPDES permitting under the Clean Water Act. Expert systems can identify chemicals that have potential adverse ecological and health effects and can help identify substances encountered in the analysis of pollutants and predict their fate in water.
 APPROACH: AI/ES programs will be integrated with some of the most widely used water quality models to facilitate data handling and the interpretation of model output for assessing the impacts of wastewater discharges. ES concepts will initially be applied to QUAL-II. A seminar-workshop will be conducted to help develop ORD and Program Office AI/ES capability and to demonstrate the utility of ES technology. An expert system will be developed to estimate transformation of pollutants and later for hydrolysis and other processes. ES ph concepts will also be applied to screen chemical structures for potential carcinogenicity.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Cooperative work by Mr. Thomas Barnwell and Dr. Linfield Brown continues in the development of an expert system application package for the QUAL2E model.

An ORD/Program Office workshop on AI languages was held in Athens on June 7-10. Dr. Don Nute of the University of Georgia's Advanced Computational Methods Center led the workshop, which included a 2-day PROLOG tutorial.

The implementation of all the program elements of an expert system for analyzing the zone of initial dilution in waters receiving pollutants has been completed. A paper describing the work, "Expert System for Mixing Zone Analysis of Toxic and Conventional Discharge," has been prepared for the National Con-

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

ference on Hydraulic Engineering in August.

A paper entitled "Uncertainty Analysis in Water Quality Modeling Using QUAL2E" (7157B) was prepared for publication in the proceedings of the 1st Symposium on System Analysis in Water Quality Management, June 30, 1987, London England.

Dr. Linfield Brown presented a paper, "An Expert Advisor for the QUAL2E Model," at the spring AGU meeting in Baltimore.

Drs. Anil Nerode and Wiktor Marek, experts on knowledge engineering and expert systems, are working with Ron Mosely of ERL/RTP on an expert system for radon contamination through the cooperative agreement with University of Pittsburgh.

SCHEDULE AND STATUS OF DELIVERABLES:

7161 EXPERT SYSTEM FOR ASSESSMENT OF THE ZONE OF INITIAL
DILUTION (ZID) AND THE MIXING ZONE IN RIVERS.
DUE: 03/31/87 REVISED: 03/31/88 COMPLETED: 01/01/00

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

CODE TITLE

BUDGET SUB-ACTIVITY: B101 WATER
ISSUE: A WQBA/PERMITTING
PPA (L): 16 WETLANDS RES. ON WQ, MITIGATION & CUMULATIVE EFFECTS OF LOSS
PPA (S): 16 WETLANDS
RC: K ERL ATHNS
PROJECT: 01 Predictive Models for Evaluating WQ Benefits of Wetlands
PROJECT OFFICER: Harvey W. Holm PHONE: FTS-250-3103

***** PLANNED START: 06/01/86 PLANNED END: 09/30/90 *****

PROJECT DESCRIPTION:

GOAL: To develop a modeling technique for evaluating the water quality benefits provided by wetland ecosystems.
RATIONALE: Wetlands, primarily through actions of microbial communities, provide environmental benefits by capturing organic toxicants and heavy metals. This pollution control function must be evaluated and documented so that the beneficial effects of wetlands in water quality maintenance can be evaluated against the economic value of land development.
APPROACH: The microbiological community ecodynamics that create toxicant dissimilation capacities and the environmental chemodynamics of heavy metals will be characterized. This will include investigation of the effects of geographic and seasonal variables on process dynamics, the interactions of nutrient and toxicant loadings, and the load-bearing capacities of wetlands. This information along with other AERL work in ecological risk analysis will be used to develop a nutrient-organic toxicant-heavy metal computer model that can objective tool for rational risk/benefit evaluations in specific wetland dision ma basins. an

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A draft design report on the decision support system for regulation based on water quality functions of freshwater wetlands (7487A) was completed by Mike Timpe. The primary objective was to develop an integrated system that is flexible enough to accommodate continuing expansion and future development, while delivering state-of-the-art analytical simulation capabilities. Other activities were:

1. Analysis of Functional Objectives. (Objective: Determination of suitable input data and definition of the information to be generated by the software.) Distribution of the draft design report should generate useful comments. Timpe presented an information seminar to the Risk Assessment group describing the overall software systems development from the perspectives of the wetlands pro-

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THIRD QUARTER STATUS REPORT ON FY'87 PROJECT DESCRIPTIONS
 OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
 ERL ATHNS: APRIL - JUNE 1987

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

ject and its defined objectives, as well as the larger view of EPA's simulation modeling development strategies in general. Burns and Timpe participated in an EPA/NASA meeting to explore potential for joint user applications for routine usage of remote sensing data.

2. Database Management and GIS Interface. (Objective: Construction of software for management of natural resource datasets with interface software for Geographic Information Systems (GIS), simulation models and graphical outputs.) Timpe performed some initial cleanup and test compilations of the ANNIE and WDM (Watershed Database Management System) routines. A summary overview of the current system was included in the design report. Timpe participated in a work session to focus on the detailed incorporation of graphics standards and the mechanics of the WDMS/GIS interface, and is currently reviewing a large commercial graphics library (RPA CAPLIB) for potential conversion to the WDMS system. The software would support the GIS graphics standard, and would become public domain. Timpe participated in the ERDAS User's Group Meeting April 9-10 to learn more about the range of applications to which image processing technology is being applied. A number of users have successfully applied the technology to the solution of problems similar to those we face in our research program, and we should benefit significantly from their experience.

3. Simulation Models. (Objective: To assemble and code ecological models to describe the water quality benefits of wetland ecosystems and place them in a landscape context for the evaluation of their public value and replacement costs.) Timpe performed a maintainability analysis on the EXAMS program at EPA's National Computer Center with the Maintainability Analysis Tool (MAT). The output from this analysis indicated some real or potential problems in the code, which were investigated and corrected as needed, for production of an up-grade version of EXAMS. Work is proceeding to produce a minimal superset from the existing COMMON blocks in HSPF prior to applying the MAT static analysis. Completion of this large task will maximize the useful information from the MAT analysis and will lay the groundwork for future program modification. The complete library of available microcomputer software was obtained from the Army Corps of Engineers Hydrologic Engineering Center. A number of these packages are candidates for adaptation. In particular, HEC-1 Flood Hydrograph Package, HEC-2 Water Surface Profiles, and HYDPAR Hydrologic Parameters can provide useful services for a wetlands modeling system.

4. Field Investigations. (Objective: Collaborative research with ongoing wetlands research projects designed to test database management systems and simulation models, and provide data to assist in model development.) Arrangements for the "northern wetlands mesocosms" mandated by the ERL-Corvallis "Wetlands Research Plan" were begun this quarter; an IAG with USGS for work at a St. Joseph, MN, wetland was submitted in June. A cooperative agreement to contribute agreed upon funds to the Des Plains River Study will be submitted in

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THIRD QUARTER STATUS REPORT ON FY'87 PROJECT DESCRIPTIONS
 OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
 ERL ATHNS: APRIL - JUNE 1987

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

July.

SCHEDULE AND STATUS OF DELIVERABLES:

- # 7487 Report on design of a decision support system for regulation based on Water Quality functions of freshwater wetlands.
 DUE: 12/31/86 REVISED: 06/30/87 COMPLETED: 06/30/87
- # 7489 Process-based ecosystem model of water quality functions of freshwater wetlands.
 DUE: 09/30/87 REVISED: 01/31/89 COMPLETED: 01/01/00

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THIRD QUARTER STATUS REPORT ON FY'87 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

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CODE      TITLE
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BUDGET SUB-ACTIVITY: B101  WATER
ISSUE: C      WASTE WATER TREATMENT TECHNOLOGY
PPA (L): 46    INDENT. OF TOXIC CHEMICALS IN INDUSTRIAL EFFLUENTS

PPA (S): 46    TOXICS IDENT.
RC: K      ERL ATHNS
PROJECT: 02    Identify and Compile Data on Occurrence of Organics
PROJECT OFFICER: John M. McGuire      PHONE: FTS-250-3185
*****
PLANNED START: 10/01/82    PLANNED END: 09/30/90
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PROJECT DESCRIPTION:

GOAL: This research will identify and determine distribution of unlisted chemicals in industrial wastewaters. Compounds that can be identified by empirical mass spectra matching as well as those that elude identification by this technique will be included.

RATIONALE: The current list of pollutants that are regulated in industrial wastewaters was established without accurate knowledge of actual occurrence of chemicals in the wastewaters; hence, some listed compounds may occur infrequently and other hazardous or toxic chemicals that are not listed may occur more frequently than listed ones. Determining the distribution of unlisted hazardous and toxic chemicals will permit establishment of improved lists for regulation.

APPROACH: Computer programs will be developed and applied to search stored GC/MS data from industrial wastewater samples for nonpriority pollutants; mass spectra will be compared with library spectra for identification. Compounds of samples using multi spectral techniques (low resolution electron impact MS, low resolution chemical ionization MS, high resolution MS, Fourier transform infrared spectrometry). Computerized multi spectral interpretation approaches

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

An invited paper on the rubber industry phase of the Industrial Technology Division Tape Study was presented by Dr. J. M. McGuire at the Tenth Analytical Symposium, sponsored by ITD. The paper covered the tape processing approach and summarized results reported to ITD last quarter.

Last quarter, it was mentioned that the Office of Water needed additional sample information in Tape Study reports. In implementing this request, two very significant problems were found in sample identifications and GC/MS analysis conditions. The first problem was that many 1982-1983 GC/MS runs that apparently had been identified by ITD contractors as unknowns were actually quality control spikes and standards. Programs were written to solve this

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THIRD QUARTER STATUS REPORT ON FY'87 PROJECT DESCRIPTIONS
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ERL ATHNS: APRIL - JUNE 1987

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:
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problem, and we can now identify these quality control samples. The second problem was that a large fraction of the 1983-1986 runs did not follow the recommended analytical protocols. Because of the multiple deviations from the protocols, standard deviations of raw GC relative retention times have increased by an order of magnitude compared to old runs made using established protocols. Two means of resolving this problem are being investigated.

Programs were written to convert the John Wiley collection of mass spectra of 110,000 compounds into a library for the ITD Tape Study. Initial results are very encouraging; however, the new library has led to several error messages that are not understood as yet.

Statistics on the frequency of occurrence in the early Effluent Guidelines Division Tape Study of carcinogenic compounds from the National Cancer Institute listings were furnished to OEPER for the Office of Technology Assessment. The request was from Karl Kronebusch of OTA.

A variety of instrument problems were experienced. A lightning bolt shut down the VAX for a few days and the modem connections for a longer time. The SS200 interface for the CH5-DF developed major problems, which are not yet resolved. Read-out errors in the MAT-44S mass spectrometer were found to be due to failure of obsolete components for which no substitutes are approved. Replacement with components having similar characteristics seems to have been successful.

SCHEDULE AND STATUS OF DELIVERABLES:

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# 7577 REPORT ON TAPE STUDY OF UP TO 6000 GC/MS SAMPLE RUNS. (K)
DUE: 11/30/87 REVISED: 01/01/00 COMPLETED: 01/01/00

# 7578 REPORT ON CONFIRMATION OF TENTATIVE IDENTIFICATIONS OF COMPOUNDS
IDENTIFIED BY SPECTRA MATCHING. (K)
DUE: 03/30/88 REVISED: 01/01/00 COMPLETED: 01/01/00

# 7579 REPORT ON MULTI SPECTRAL IDENTIFICATIONS OF MIS LIB COMPOUNDS. (K)
DUE: 12/30/88 REVISED: 01/01/00 COMPLETED: 01/01/00

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

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CODE      TITLE
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BUDGET SUB-ACTIVITY: D109  HAZARDOUS WASTE-NONENERGY
ISSUE: C      WASTE CHARACTERIZATION
PPA (L): 28   LAND DISPOSAL BANNING ASSESSMENT AND EVAL OF OTHER MGMT SYST

PPA (S): 28   LAND DISP BANNING
RC: K        ERL ATHNS
PROJECT: 03   Measure Rate Constants and Partition Coefficients
PROJECT OFFICER: Jackson Ellington  PHONE: FTS-250-3197
*****
PLANNED START: 10/01/85  PLANNED END: 12/31/99
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PROJECT DESCRIPTION:

GOAL: Provide accurate rate constants of known precision for implementing the Hazardous Waste Management Amendments, including evaluating waste management and treatment needs based on potential human health and environmental impacts. RATIONALE: Current regulatory activities including RCRA Reauthorization requirements relative to Land Disposal Evaluation are demonstrating the lack of consistent methods and data for determining the health and environmental impact of various regulatory options. Accurate pollutant degradation rate constants of known precision are needed for more scientifically sound and consistent decision-making on waste management options. APPROACH: Experimental techniques will be adapted or developed, standardized, and applied to measure degradation rate constants and partition coefficients for selected organic chemicals. Measured and literature information will be incorporated into computerized data bases for use with multimedia models for evaluating waste management and treatment needs relative to the Land Disposal Evaluation.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

During the quarter, measurements were completed for the remainder of the hydrolysis rate constants and octanol/water partition coefficients for which data were missing in the "second third" of the Appendix VIII compounds being evaluated under the land decision rule. Identities of the compounds measured were confirmed by mass spectrometry and infrared spectrometry. Data are published in two reports: "Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Rate Constants for Evaluation of Hazardous Waste Land Disposal: Volume II. Data on 54 Chemicals," (7686A) by J. Jackson Ellington; Frank E. Stancil, Jr.; William D. Payne; and Cheryl Trusty, and "Octanol/Water Partition Coefficients for Evaluation of Hazardous Waste Land Disposal: Part 2. 'Second Third' Chemicals," (7687A) by Ellington and Stancil.

A poster session, "Use of Standard Reference Compounds to Assure Comparison of Hydrolysis Rate Constant Measurements," by Ellington, Stancil and Payne, was presented at the 17th Annual Symposium on the Analytical Chemistry of Pollutants, May 18-20, 1987.

A literature survey for hydrolysis rates and octanol/water partition coefficients is underway for compounds without measured values in the Appendix VIII "third third" and for compounds under consideration in the concentration based listing project.

SCHEDULE AND STATUS OF DELIVERABLES:

- # 7686 SECOND REPORT ON HYDROLYSIS RATE CONSTANTS FOR LAND BANNING
DECISION RULE.
DUE: 05/30/87 REVISED: 01/01/00 COMPLETED: 05/30/87
- # 7687 SECOND REPORT ON PARTITION COEFFICIENTS FOR LAND BANNING
DECISION RULE.
DUE: 05/30/87 REVISED: 01/01/00 COMPLETED: 05/30/87

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

bility of Hydrolysis Rate Constant Measurements," by Ellington, Stancil and Payne, was presented at the 17th Annual Symposium on the Analytical Chemistry of Pollutants, May 18-20, 1987.

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ERL ATHNS: APRIL - JUNE 1987

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CODE      TITLE
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BUDGET SUB-ACTIVITY: D109  HAZARDOUS WASTE-NONENERGY
ISSUE: C      WASTE CHARACTERIZATION
PPA (L): 28    LAND DISPOSAL BANNING ASSESSMENT AND EVAL OF OTHER MGMT SYST

PPA (S): 28    LAND DISP BANNING
RC: K          ERL ATHNS
PROJECT: 07    Environmental Process Characterization - Metals
PROJECT OFFICER: Arthur W. Garrison      PHONE: FTS-250-3145
*****
PLANNED START: 10/01/84    PLANNED END: 12/31/99
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PROJECT DESCRIPTION:

GOAL: Provide data on fate and transport of toxic metals for development of exposure assessment models for implementing the Hazardous Waste Management Amendments, including evaluating waste management and treatment needs based on potential human health and environmental impacts.

RATIONALE: Current activities including RCRA Reauthorization requirements relative to Land Disposal Evaluation demonstrate the lack of consistent exposure assessment methods and data for determining the health and environmental impact of various regulatory options. Data on fate and transport of toxic metals are needed for inclusion in models for exposure assessment.

APPROACH: Thermodynamics and kinetics of sorption of metal cations, metal-ligand complexes and other metal species on soils, sediments, and aquifer substrates will be studied. Specific sorbates will include minerals, organic-coated minerals, and dissolved humic materials. Distribution coefficients will be determined using plasma emission spectroscopy. Kinetic equations and equilibrium constants will be determined and categorized for use in exposure and risk models.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Work on the "accelerated metals plan" for OSW this quarter included: 1) meeting with OSW and its contractor to plan collection of aquifer samples necessary for much of this accelerated work, 2) continued inhouse development of concepts, models, and databases for improved sorption terms for the MINTEQ model for fate of metals in groundwater, 3) performance of initial experiments for estimation of distribution coefficients between metals and aquifer solids, and 4) assembly of funding packages for the various extramural efforts supported by OSW through ERL-Athens. Funds were added to a cooperative agreement between ERL-Ada and Colorado School of Mines (CSM) for work on redox measurements in aquifer systems; work has already begun. CSM also has begun work to identify organic complexation agents in leachates and determine their stability constant with metals of interest to OSW. A literature-derived data base of this informa-

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ERL ATHNS: APRIL - JUNE 1987

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

tion is being incorporated into MINTEQ by ERL-Athens. A database of stability constants for metal-hydrous oxide interactions was obtained from Carnegie Mellon University; this has also been adapted for use in MINTEQ modeling. Aquifer samples collected by the OSW contractor will begin arriving at ERL-Athens about mid-August.

In in-house research, competitive adsorption of 14 metals on 4 clay minerals--montmorillonite, kaolinite, illite, and vermiculite--was completed. Kaolinite showed negative adsorption at pH 4 for all metals except Cr. Montmorillonite and illite exhibited no preferential sorption of any divalent transition metal cation, but vermiculite exhibited some preferential sorption. For these clays, the order of sorption onto a sodium-saturated clay was $M+3 > M+2 > M+1$. Studies using the same above systems and calcium (40 ppm), cysteine and a combination of both as desorbing agents also were completed.

Two scientists from the People's Republic of China are working inhouse under a PRC-US agreement--one on metal-humic interactions and one on metal-sulfide mineral interactions. They are beginning to produce results that contribute to the goals of this project.

A reverse osmosis sampling system was developed, tested, and used on-site by Georgia Institute of Technology personnel to collect and concentrate by twenty-fold 200g of dissolved organics in Suwannee River (Okefenokee Swamp) water. Ninety-five percent recovery of total dissolved organics was obtained. This organic material will be fractionated to provide the necessary quantity of fulvic and humic acids for use by Georgia Tech, University of Georgia, and inhouse researchers studying metal-organic interactions.

Work continues at the University of Georgia on use of laser-excited lanthanide ion fluorescence for characterization of metal binding sites in humic materials. Several experiments were completed to establish the precision and accuracy of the recently installed spectrometer system. These included experimental measurement of the emission spectra and lifetimes of Eu(III). Most importantly, confirmation of earlier experimental results on the binding of Eu(III) by humic acid was attained.

Inhouse work involving multielement analysis of groundwater/aquifer sample for determination of distribution coefficients of metallic elements between ground-water and aquifer solids was completed. This work has established a unique background of experience that will be extremely useful in the next few months when aquifer samples from sites throughout the United States will be shipped to ERL-Athens for determination of metal-aquifer solid distribution coefficients and testing of the MINTEQ predictive model.

SCHEDULE AND STATUS OF DELIVERABLES:

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ERL ATHNS: APRIL - JUNE 1987

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SCHEDULE AND STATUS OF DELIVERABLES:

# 7350	ARTICLE ON THE KINETICS OF SORPTION AND DESORPTION OF METALS IN SUBSURFACE ENVIRONMENTS DUE: 07/31/89 REVISED: 01/01/00 COMPLETED: 01/01/00
# 7351	ARTICLE DESCRIBING KINETICS OF COMPLEXATION PHENOMENON FOR METALS IN AQUEOUS SYSTEMS DUE: 07/31/89 REVISED: 01/01/00 COMPLETED: 01/01/00
# 7691	REPORT ON DISTRIBUTION COEFFICIENTS OF METALS SORBED TO AQUIFER SUBSTRATES. (K) DUE: 01/30/87 REVISED: 01/01/00 COMPLETED: 01/30/87
# 7692	REPORT ON METAL BINDING TO HUMIC/FULVIC MATERIALS. DUE: 08/30/87 REVISED: 01/01/00 COMPLETED: 01/01/00
# 7693	REPORT ON LASER SPECTROMETRY APPLIED TO METAL-ORGANIC SPECIATION IN WATER. (K) DUE: 12/30/86 REVISED: 01/01/00 COMPLETED: 12/31/86

DATE: 8/13/87

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

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***** EARTHNS: APRIL - JUNE 1987 *****
CODE      TITLE
BUDGET SUB-ACTIVITY: D109  HAZARDOUS WASTE-NONENERGY
ISSUE: C      WASTE CHARACTERIZATION
PPA (L): 28    LAND DISPOSAL BANNING ASSESSMENT AND EVAL OF OTHER MGMT SYST
PPA (S): 28    LAND DISP BANNING
RC: K          ERL ATHNS
PROJECT: 17    Environmental Process Characterization (Biological)
PROJECT OFFICER: John E. Rogers      PHONE: FTS-250-3592
*****
***** PLANNED START: 03/01/85 ***** PLANNED END: 12/31/99 *****

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PROJECT DESCRIPTION:

GOAL: Provide integrated (multimedia) methods and data for implementing the Hazardous Waste Management Amendments, including evaluating waste management and treatment needs based on potential human health and environmental impacts.

RATIONALE: Current regulatory activities including RCRA Reauthorization requirements relative to Land Disposal Evaluation are demonstrating the lack of consistent methods and data for determining the health and environmental impact of various regulatory options. Integrated (multimedia) methods that accommodate knowledge of uncertainty are needed for more accurate and consistent decision-making on waste management options.

APPROACH: Mechanisms of anaerobic biotransformations of xenobiotic chemicals will be characterized using kinetic equations. Laboratory studies will be conducted to test these models and to identify environmental parameters that impact the rates and extent of the biotransformation processes.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A manuscript, "Microbial Transformation Rates of High Concentrations of Toxic Organic Chemicals in Natural Streams" (Huang, Hodson and Lewis) (7347B) was submitted to Applied and Environmental Microbiology. Research on the toxicity of high concentrations of toxic organic chemicals in natural streams is being carried out through the UGA Cooperative Agreement, Subproject 3. This research is designed to evaluate the validity of assuming no microbial degradation in toxic waste sites where one or more chemicals exist at concentrations toxic to general microbial metabolic processes.

Dr. Rogers was asked to chair a session entitled "Anaerobic Biodegradation of Xenobiotic Compounds" at the SETAC 8th Annual Meeting, November 9-12, 1987, Pensacola, FL. He also was asked to chair a session on the biological treatment of hazardous waste as part of the Symposium on Chemical and Biological Detoxification of Hazardous Waste at the American Chemical Society Meetings, New Orleans, LA, August 30-September 4, 1987.

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ERL ATHNS: APRIL - JUNE 1987

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The organic chemicals reported in Table C-5 on page 21675 of the Federal Register Vol 51, No. 114, were evaluated for their relative biodegradability in subsurface environments. The compounds were subsequently divided into three groups as a result of the evaluation. The three groups were: (1) compounds for which laboratory data should be immediately developed because their rates of degradation may be fast enough to significantly impact the output of mathematical models used in regulatory processes; (2) compounds for which there is a marginal chance that laboratory data would impact regulatory processes, and (3) compounds for which anaerobic degradation that should not be considered because their degradation will be too slow to have an effect.

Following up on our previous studies of the degradation of dichlorophenols in anaerobic sediments, we have taken a closer look at the assay procedures that we have been using. The extrapolation of laboratory data to the field is highly dependent on knowing the relationship between the true environmental rate and the rate of degradation determined in the laboratory. In this regard we are currently investigating the effect of dilution of the sediment samples and the effect of varying the sediment sample size while maintaining a constant sediment-to-water ratio. As the ratio of sediment to water was increased from 1:5 to 1:100 a large increase was observed in the lag period before degradation could be detected. Apparently the less dilute the sample, the more likely that it represents the environmental rate of degradation. From a practical sense, however, if conservative rates are needed as input for current regulatory models, the more dilute assays would be preferred.

We have also initiated studies in the following three areas:

(1) We are currently examining the degradation of a series of dichlorinate anilines in anaerobic sediments as a parallel study to the one currently being conducted with dichlorophenols. We hope to determine whether we are dealing with only a few organisms with broad substrate specifications for degrading dichlorophenols or a wide variety of organisms with very specific substrate specificities. We will also be looking at the difference between static and shaken assays.

(2) We are extending the studies initiated by a visiting Soviet scientist, Dr. N. D. Ananyeva, who was investigating the adaptation period that generally occurs in natural waters and sediments before degradation can be detected by investigating the degradation of phenol, p-cresol, a-naphthol and quinoline in natural waters. Results from these studies will be reported at the SETAC meeting this fall and at the American/Soviet Symposium to be held in Iowa City this October.

(3) As part of a cooperative agreement with the University of Georgia,

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the temperature dependence of the degradation of xenobiotics in anaerobic environments is being investigated. The dechlorination of 2,4-dichlorophenol in sediments amended with 2000 ppm sulfate was recently observed. Sulfate has been reported to inhibit this reaction in some sediments.

SCHEDULE AND STATUS OF DELIVERABLES:

7690 INTERNAL REPORT ON EQUATION FOR PREDICTING ANAEROBIC TRANSFORMATIONS WITHIN
THE SATURATED ZONE
DUE: 07/31/89 REVISED: 11/30/89 COMPLETED: 01/01/00

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

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CODE      TITLE
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BUDGET SUB-ACTIVITY: D109  HAZARDOUS WASTE-NONENERGY
ISSUE: C      WASTE CHARACTERIZATION
PPA (L): 28    LAND DISPOSAL BANNING ASSESSMENT AND EVAL OF OTHER MGMT SYST
PPA (S): 28    LAND DISP BANNING
RC: K      ERL ATHNS
PROJECT: 21    Multimedia Modeling with Uncertainty Analysis
PROJECT OFFICER: Lee A. Mulkey      PHONE: FTS-250-3160
*****
PLANNED START: 09/01/85    PLANNED END: 12/31/99
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PROJECT DESCRIPTION:

GOAL: Provide multimedia methods complete with uncertainty analysis capabilities for implementing the Hazardous Waste Management Amendments including evaluating waiver petitions, listing procedures, and delisting petitions based on human health and environmental impacts.

RATIONALE: Current regulatory activities including RCRA Reauthorization requirements relative to Land Disposal Evaluation are demonstrating the lack of consistent methods and data for determining the health and environmental impact of various regulatory options. Integrated (multimedia) methods that accommodate knowledge of uncertainty are needed for more accurate and consistent decision-making on waste management options.

APPROACH: The decision rule model will be subjected to a series of tests with various measurement errors assumed for the inputs. OSW staff will be consulted on outcomes to evaluate impact of input accuracies on resulting rule decisions to define acceptable experimental accuracy. The range of environmental appropriate. Multimedia models capable of simulating both the engineering and u controls and post-closure performance will be developed for use in evaluating banning waiver requests.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The report describing the multimedia modeling for hazardous wastes, "Multimedia Exposure Assessment Model for Evaluating Land Disposal of Hazardous Wastes: A Progress Report," (6015A) was completed. The computer code was delivered and it is currently undergoing testing and evaluation. OSW was provide a copy and their staff is conducting sensitivity analysis. A major question under investigation is the role of the unsaturated zone on downgradient exposures. In its current form, the model includes vapor and leachate fluxes to the atmosphere and soil, fate in the unsaturated zone, fate in the saturated zone, and plume interception by surface water and subsequent water quality fate

The diffuse layer metal sorption model algorithm developed by David

continued...

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Dzombak at MIT was incorporated into the MINTEQA1 model code. This sorption model is expected to improve our ability to model metal-bearing leachates from land disposal systems.

Two new projects were initiated this quarter. The first, Development of a Site Specific Version of the Multimedia Exposure Model, will consist of two primary efforts: integration of a numerical unsaturated/saturated code as an option to the current analytical scheme, and development/implementation of an alternative scheme for the monte carlo approach to uncertainty analyses. With these enhancements, the model will be capable of incorporating site-specific spatial variability and be able to efficiently perform uncertainty analysis. The second, Development of a Coupled Metal Speciation-Transport Model, will produce a prototype model for simulating metals movement in porous media. A key element of the approach is the use of MINTEQA1 to specify the minimum number of reactions and thermodynamic constants required in any given analyses so that computational burdens can be alleviated.

ERL-Athens and OSW are performing a comprehensive set of sensitivity analyses with the suite of exposure models used for land disposal regulation. Impacts of anaerobic degradation, alternative formulations for dispersivity, the unsaturated zone depths, and hydrolysis rate constants are being evaluated for 44 chemicals.

SCHEDULE AND STATUS OF DELIVERABLES:

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# 6015  Report on Organics Multi Media Human Exposure Model
      DUE: 09/30/86  REVISED: 05/31/87  COMPLETED: 05/31/87

# 7352  PROJECT REPORT ON PERFORMANCE TESTS OF OSW MODELING
      APPROACH USING FIELD DATA
      DUE: 11/30/87  REVISED: 02/29/88  COMPLETED: 01/01/00

# 7353  REPORT ON EVALUATION OF LAND DISPOSAL SYSTEMS, PROJECT
      DESIGNS AND ASSESSMENT OF THEIR FAILURE PROBABILITIES
      DUE: 04/30/88  REVISED: 01/01/00  COMPLETED: 01/01/00

# 7684  PROJECT RPT. ON UNCERTAINTY ANALYSIS OF MULTIMEDIA (AIR, UNSATURATED ZONE,
      GROUND WATER), TRANSIENT-FINITE SOURCE, LAND DISPOSAL MODEL.
      DUE: 09/30/87  REVISED: 01/01/00  COMPLETED: 01/01/00

# 7685  USERS MANUAL FOR MULTIMEDIA, TRANSIENT, LAND DISPOSAL MODEL.
      DUE: 02/28/88  REVISED: 01/01/00  COMPLETED: 01/01/00

# 7694  USER'S MANUAL FOR METAL SPECIATION MODELING - MINTEQ.
      DUE: 03/30/87  REVISED: 01/01/00  COMPLETED: 03/30/87

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: APRIL - JUNE 1987

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CODE      TITLE
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BUDGET SUB-ACTIVITY: D109    HAZARDOUS WASTE-NONENERGY
ISSUE: C      WASTE CHARACTERIZATION
PPA (L): 28    LAND DISPOSAL BANNING ASSESSMENT AND EVAL OF OTHER MGMT SYST
PPA (S): 28    LAND DISP BANNING
RC: K      ERL ATHNS
PROJECT: 38    Environmental Process Characterization - Organics
PROJECT OFFICER: N. Lee Wolfe    PHONE: FTS-250-3429
*****
PLANNED START: 10/01/84    PLANNED END: 12/31/90
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PROJECT DESCRIPTION:

GOAL: Provide data on fate and transport of anthropogenic organic compounds for development of exposure assessment models for implementing the Hazardous Waste Management Amendments, including evaluating waste management and treatment needs based on potential human health and environmental impacts.

RATIONALE: Current activities including RCRA Reauthorization requirements relative to Land Disposal Evaluation demonstrate the lack of consistent exposure assessment methods and data for determining the health and environmental impacts of various regulatory options. Data on fate and transport of anthropogenic organic compounds are needed for inclusion in models for exposure assessment.

APPROACH: Detailed laboratory kinetic studies will be conducted to describe soil mediated hydrolysis and abiotic redox transformation reactions of organics as a function of pH and redox potential in the sorbed and bulk aqueous phase of soil-water systems. Molecular and system variables that govern redox and other processes will be related and quantified.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Nitrobenzene reduction studies were extended to soil-water samples obtained from two aquifers. The disappearance rate constants are approximately five times slower in the aquifer samples than in sediment samples collected in the Athens area. Detailed concentration studies of substituted nitrobenzenes indicated that the disappearance rate constants were dependent on the initial concentration of the nitrobenzene derivative. Additional studies are in progress to determine the rate limiting step of the reduction process.

Redox studies were performed on two carbamate pesticides, Protham and Carbaryl, in an anaerobic sediment/water system containing 10% solids. Kinetic results are being interpreted; decay products of these two pesticides will be analyzed. In addition to these redox studies, the hydrolysis of chlorinated

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

organic compounds is currently being investigated.

Studies of the degradation of synthetic dyestuffs in anaerobic sediments continue. The effects of pH on the distribution and kinetics of reduction were studied for a nonionizable dye, azobenzene, and an ionizable dye, Congo Red. Results indicate that pH will have little effect on the distribution and reduction of azo dyes containing non-ionizable functional groups. For those dyes that do contain ionizable groups, pH will play an important role in their distribution and, thus, transport in natural systems. Changes in pH, however, may have little effect on the rate of reduction of these dyes at the sediment-water surface.

Studies on sorption of ionizable organic compounds to soils, sediments and aquifer material continue. Experimental work confirms that partitioning of the anion of pentachlorophenol (pentachlorophenolate) between octanol and water is highly dependent on ionic strength of the water phase and that partitioning of both the ion-paired phenolate and free phenolate species into octanol is important.

A workshop on the Environmental Chemistry of Dyes, organized by the Athens Laboratory, has been tentatively scheduled for November 12-13, 1987, in Pensacola, FL. A symposium entitled "Environmental Chemistry of Ionic Xenobiotics," also organized by the Athens Laboratory, will be held at the SETA conference.

SCHEDULE AND STATUS OF DELIVERABLES:

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# 7349  ARTICLE ON THE ROLE OF SOIL IN MEDIATING THE HYDROLYSIS
        OF ORGANIC COMPOUNDS
        DUE: 09/30/88    REVISED: 01/31/89    COMPLETED: 01/01/00

# 7688  JOURNAL ARTICLE ON ABIOTIC REDOX REACTIONS IN SEDIMENT-SOIL
        SYSTEMS (K)
        DUE: 10/30/86    REVISED: 01/01/00    COMPLETED: 10/30/86

# 7689  REPORT DESCRIBING THE KINETICS OF REDOX REACTIONS IN SOIL-WATER
        ENVIRONMENTS
        DUE: 12/30/88    REVISED: 04/30/89    COMPLETED: 01/01/00

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 OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
 ERL ATHNS: APRIL - JUNE 1987

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CODE      TITLE
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BUDGET SUB-ACTIVITY: D109    HAZARDOUS WASTE-NONENERGY
ISSUE: D      DIOXIN
PPA (L): 54    MOVEMENT AND PERSISTENCE OF DIOXINS IN SOILS AND GROUNDWATER

PPA (S): 54    DIOXIN TRANSPORT
RC: K          ERL ATHNS
PROJECT: 35    Photodegradation of Dioxin in Soils
PROJECT OFFICER: Richard G. Zepp    PHONE: FTS-250-3428
*****
PLANNED START: 10/01/85    PLANNED END: 12/31/99
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PROJECT DESCRIPTION:

GOAL: Provide OSWER with techniques and necessary data to predict the rate and extent of movement and transformations of 2,3,7,8-tetrachlorodibenzo-p-dioxin in soils and in ground waters.

RATIONALE: These data are necessary to assess the potential for human exposure to dioxin and to make rational decisions regarding the removal and disposal of dioxin-contaminated soils. These data will also aid in the development of technologies to desorb dioxin from soils and to detoxify dioxins in contaminated soils.

APPROACH: Studies will be conducted to determine equations and rate constants that describe the photolysis of dioxins on soils. The studies will examine direct photolysis as well as indirect photoprocesses involving light-generated oxidizing species on soil surfaces.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Research continues at the University of Nevada-Reno on photolysis and other environmental reactions of various dioxins on soil and other surfaces. Efforts in the past 3 months have centered on validation of previous findings of 2,3,7,8-TCDD formation from contaminated octachlorodibenzodioxin (OCDD) soils in sunlight. Soils from contaminated sites in Oregon are presently being irradiated both in the laboratory and under environmental conditions. These irradiated samples will be sent to Cal-Enseco Labs for complete isomer analysis at the end of the exposure periods. A study also is being conducted in the laboratory on two OCDD-fortified, air-dried agricultural soils to determine the depth dependence of photolysis.

Recent results from irradiating 2,3,7,8-TCDD fortified soils with hydrogen donating solvents support previous studies that oil additives increase the rate of photolysis. Future studies will determine whether this is a result of transport or photochemistry.

SCHEDULE AND STATUS OF DELIVERABLES:

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 ERL ATHNS: APRIL - JUNE 1987

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SCHEDULE AND STATUS OF DELIVERABLES:

7355 REPORT ON PHOTODEGRADATION EVALUATION OF DIOXIN (2,3,7,8-TCDD) IN SOILS
 DUE: 06/30/88 REVISED: 09/30/88 COMPLETED: 01/01/00

CLIENT OFFICE:

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ERL ATHNS: APRIL - JUNE 1987

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CODE      TITLE
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BUDGET SUB-ACTIVITY: E104  PESTICIDES NCNENERGY
ISSUE: D      ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION
PPA (L): 07    GROUNDWATER: PEST. CONTAMINATION AND PROCESS STUDIES

PPA (S): 07    PEST. GROUNDWTR RES.
RC: K          ERL ATHNS
PROJECT: 24     Validation of Predictive Techniques for Environ. Exposure
PROJECT OFFICER: Robert F. Carsel      PHONE: FTS-250-3138
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PLANNED START: 04/01/81    PLANNED END: 03/31/89
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PROJECT DESCRIPTION:

GOAL: Refine, parameterize and evaluate via field and other studies the capability of single and multimedia pesticide exposure models that predict the multimedia and intermedia transport and fate of pesticides, especially through soils (including an evaluation of their leaching potential), sediments, and other porous media to ground and surface waters.

RATIONALE: Optimum pesticide regulation requires field-evaluated assessment techniques to assure that scientifically defensible decisions are made using cost-effective data specifications and assessment methods.

APPROACH: As single and multimedia pesticide exposure assessment packages are developed or assembled from SOA components on application/drift, runoff, leaching, surface stream, river and lake models, etc., and become operational, they will be systematically evaluated via application to "real world" OPP and state problems and/or by retrospective comparison studies. Limited special field studies will also be initiated in concert with OPP, states, regions, packages or specific components. Current emphasis is on the Dougherty Plain leaching study. Quality assurance activities will be conducted by Athens ERL.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Two pesticides, aldicarb and metolachlor, were successfully applied at the Dougherty Plain field site at time of planting for 1987 crop season. Application rates were monitored by both soil and filter disks. Samples were collected to evaluate composite sampling designs versus random sampling. In addition, post-application soil samples were collected to assess field degradation rates.

Three prototype multi-level monitoring wells were designed and fabricated.

The interagency agreement with the U.S. Geological Survey was approved and executed. This agreement provides for the conduct of experiments on the Dougherty Plain field site for the 1987 growing season and for the installation of additional monitoring well networks for monitoring bromide tracer movement.

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

On-the-job-training of newly hired personnel, cross-training of senior personnel, and general preparations for the up-coming sampling season at the Dougherty Plain field site is in progress. Reorganization of existing space and equipment, required as a result of the shift in methylene chloride operations, is near completion.

Soil profile characterization for the site down to 20 feet is now complete. Measured data of soil properties for 10 of the 20 primary sites include hydraulic conductivity, water retention curves, particle size distribution, and bulk density.

SCHEDULE AND STATUS OF DELIVERABLES:

- # 6909 Report on spatial variability of soil release characteristics (Dougherty Plain Site) for use in PRZM (testing)
DUE: 12/31/86 REVISED: 03/31/87 COMPLETED: 03/31/87
- # 6912 JOURNAL ARTICLE ON RESULTS OF FIELD TESTING OF PRZM LEACHING MODEL FOR COASTAL PLAIN SOILS
DUE: 03/31/87 REVISED: 12/31/87 COMPLETED: 01/01/00
- # 7593 DOUGHERTY PLAIN ANNUAL REPORT. (K)
DUE: 09/30/87 REVISED: 01/01/00 COMPLETED: 01/01/00
- # 7660 DOUGHERTY PLAIN ANNUAL REPORT. (K)
DUE: 09/30/88 REVISED: 01/01/00 COMPLETED: 01/01/00
- # 7661 FINAL DOUGHERTY PLAIN REPORT INCLUDING PESTICIDE GROUND WATER THREAT ASSESSMENT METHODOLOGY TEST RESULTS. (K)
DUE: 09/30/89 REVISED: 01/01/00 COMPLETED: 01/01/00
- # 7662 Internal Report Deep Soil Profile and Unconfined Aquifer Characteristics for Major Eastern Agricultural Regions-Crops
DUE: 09/30/88 REVISED: 01/01/00 COMPLETED: 01/01/00
- # 7664 GROUNDWATER PESTICIDES ASSESSMENT MANUAL FOR OPP, STATES, COUNTY EXTENSION PROFESSIONALS. (K)
DUE: 06/30/89 REVISED: 01/01/00 COMPLETED: 01/01/00

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CODE      TITLE
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BUDGET SUB-ACTIVITY: E104  PESTICIDES NCNENERGY
ISSUE: D      ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION
PPA (L): 08    PREDICTIVE TECHNIQUES FOR ENVIRONMENTAL EXPOSURE

PPA (S): 08    DEVELOP PRED. TECH.
RC: K      ERL ATHNS
PROJECT: 25    Predictive Techniques for Environmental Exposure
PROJECT OFFICER: Lee A. Mulkey      PHONE: FTS-250-3160
*****
PLANNED START: 10/01/81    PLANNED END: 12/31/99
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PROJECT DESCRIPTION:

GOAL: Provide long term, short turnaround, or direct single or multimedia exposure assessment technology assistance to OPP.

RATIONAL: OPP occasionally needs quick turnaround, customized model development and application assistance for high priority regulatory actions mandated under FIFRA. This effort provides a focused, coordinated body of expertise comprised of ORD and OPP agency personnel augmented by extramural specialists to meet this need on demand. It also provides the expertise to develop needed long term multimedia, site-specific exposure assessment modeling techniques.

APPROACH: Develop or assemble single and multimedia pesticide exposure assessment packages from SOA components and apply them to high priority OPP regulatory problems. Athens ERL also is responsible for generating needed agronomic/management scenarios for non-irrigated crop applications and reporting requirement to OPP. Close coordination with similar exposure/risk PMN assessments. Model development activities for OTS and OW are envisioned as required, e.g.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Testing and coding of a new numerical scheme for solving the pesticide transport equations in PR2M has been completed. The irrigation algorithms and coding was completed.

Preliminary drafts of journal articles entitled "The Effect of Aggregate Size Distribution on Solute Transport in Aggregated Media," and "Modeling of Solute Transport in Sediment Suspensions with Nonlinear Sorption Isotherms" are under review.

A major project meeting was held to coordinate details of linking the saturated zone/unsaturated zone transport codes. Key players from the primary contractor, Woodward-Clyde Consultants, and their subcontractor, Geotrans, Inc.

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

attended the meeting.

A PC version of a water treatment model was completed and a draft report/computer code is undergoing review and testing. The model allows any unit operation (e.g., sedimentation, coagulation, carbon sorption) to be converted and treatment removals computed based on chemical properties. The model will be used as part of the exposure assessment package for pesticides, toxics, and hazardous wastes.

SCHEDULE AND STATUS OF DELIVERABLES:

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# 7258 FEASIBILITY REPORT FOR UNSATURATED-SATURATED ZONE PESTICIDE
      EXPOSURE MODEL.
      DUE: 01/31/87    REVISED: 01/01/00    COMPLETED: 01/31/87

# 7695 JOURNAL ARTICLE ON SPATIAL VARIABILITY OF PESTICIDE APPLICATION. (K)
      DUE: 11/30/86    REVISED: 01/01/00    COMPLETED: 11/30/86

# 7709 Users Manual for Exposure Assessment Model of Pesticide Contamination of
      Ground Water
      DUE: 06/30/88    REVISED: 01/01/00    COMPLETED: 01/01/00

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ERL ATHNS: APRIL - JUNE 1987

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CODE      TITLE
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BUDGET SUB-ACTIVITY: E104  PESTICIDES NCNENERGY
ISSUE: I      ECOLOGY: ECOTOXICITY AND RISK ASSESSMENT
PPA (L): 13    DEVELOPMENT OF INTEGRATED RISK ASSESSMENT MODELS

PPA (S): 13    INTEGRATED RISK ASS.
RC: K          ERL ATHNS
PROJECT: 26    Risk Assessment Methods for FIFRA
PROJECT OFFICER: Lee A. Mulkey  PHONE: FTS-250-3160
*****
PLANNED START: 10/01/85  PLANNED END: 12/31/99
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PROJECT DESCRIPTION:

GOAL: Develop, refine and extend existing terrestrial and aquatic fate, transport and effects models to include hazard impact, subroutines and data for environmental risk assessments (RA) for the labeled use of pesticides. Results must be expressed in terms of probability of impact and frequency of occurrence and duration.

RATIONALE: Proven, operational environmental RA models are needed to evaluate registration requests for new pesticides and for re-registration and label changes (e.g. new uses) of existing compounds under FIFRA.

APPROACH: Existing unsaturated/saturated zone soil transport models, proven runoff-surface water pesticide codes, appropriate ground water codes and related air transport models will be combined to produce SOA exposure assessment model framework. These will then be linked with available effects models to produce defensible RA methodologies for OPP. As completed, the risk assessment packages will be tested and evaluated, especially in terms of coordination will be required with CERL, RSKERL, ASRL-RTP and the aquatic fate p research at AERL.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A new project was initiated to provide a "level 1" screening model for terrestrial exposure using analytical solutions to a set of coupled differential equations for pesticide fate and terrestrial food chain dynamics. This product to be included as an option in the prototype terrestrial exposure model, will be completed in April 1988. It will be demonstrated in a planned December workshop for OPP.

The decision was made to develop a "place-holder" model for plant uptake in the Terrestrial Environmental Exposure Assessment Model (TEEAM) until ERL-Corvallis can complete the comprehensive model. A set of program specification and coding conventions was forwarded to the Corvallis Lab for consideration.

SCHEDULE AND STATUS OF DELIVERABLES:

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SCHEDULE AND STATUS OF DELIVERABLES:

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# 7501 Initial Design and Specifications of Computerized Terrestrial
      Exposure Model
      DUE: 09/30/87  REVISED: 01/01/00  COMPLETED: 01/01/00

# 7502 SOILS AND METEOROLOGICAL DATABASES FOR TERRESTRIAL EXPOSURE MODELS
      DUE: 09/30/87  REVISED: 04/30/88  COMPLETED: 01/01/00

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CODE      TITLE
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BUDGET SUB-ACTIVITY: L104 TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY
ISSUE: D      ECOLOGY, TRANSPORT/FATE/FIELD VALIDATION
PPA (L): 09    DEVELOPMENT OF VALIDATED EXPOSURE ASSESSMENT METHODOLOGIES

PPA (S): 09    EXPOSURE ASSESSMENT
RC: K
PROJECT: 27    Development of Validated Exposure Assessment Methodologies
PROJECT OFFICER: Robert B. Ambrose      PHONE: FTS-250-3546
*****
PLANNED START: 10/01/79    PLANNED END: 12/31/99
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PROJECT DESCRIPTION:

GOAL: Develop, parameterize and evaluate a first-generation metals modeling system and continue development and modification of multimedia models for non-human exposures.

RATIONALE: O.S. wants to upgrade its metals and organics multimedia modeling capability for PMN activities and comprehensive risk/benefit analyses on the impacts of regulating existing chemicals/species and to account for potential toxic effects at the organism and systems levels given various toxics loading combinations into surface waters and other environmental compartments.

APPROACH: Thermodynamic metals species and chemical reaction models will be combined with partitioning and bioaccumulation (including plants) models to reduce a process-based aquatic distribution package for metal species. This, in turn, will be interfaced with user-friendly software and steady-state transport codes to produce MEXAMS, a first generation metals exposure assessment model. Also, additional refinements in transport codes incorporated into multimedia models to produce more reliable exposure estimates of pol assessment packages for organics of interest under TSCA and RCRA.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A competitive cooperative agreement procurement process was initiated for the development of a general fine sediment transport model. Four preproposals were selected for solicitation as full proposals.

A new project with the University of Georgia Computer Science Department was initiated to implement changes in the numerical solution procedures within MINTEQA1 and prepare detailed documentation for selected subroutines.

A manuscript entitled "Simulation Models for Waste Load Allocation of Toxic Chemicals - A State of the Art Review," was submitted to the Water Pollution Control Federation for review and publication. The paper includes procedures for both organic and metal pollutants.

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A paper entitled "Environmental Photoprocesses Involving Natural Organic Matter" (7672A) was submitted as a chapter in Humic Substances and Their Role in the Environment.

A handbook entitled "Processes, Coefficients, and Models for Simulating Toxic Organics and Heavy Metals in Surface Waters" (6949A) was completed for publication (EPA/600/3-87/015).

The manuscript entitled "Effects of Structurally Related Compounds on the Transformation of Xenobiotic Compounds in Natural Waters" (7670A) has been submitted for publication in Applied and Environmental Microbiology. This paper covers the investigation of the transformation of individual xenobiotic compounds added singly or as components of mixtures composed of structurally related compounds in natural waters. The rate of transformation of some compounds was altered in the presence of increasing concentrations of structurally related compounds.

SCHEDULE AND STATUS OF DELIVERABLES:

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6949 Project report on rates, constants, and kinetic formulations for organic
 chemicals and metals
 DUE: 12/31/86 REVISED: 04/30/87 COMPLETED: 04/30/87

7670 JOURNAL ARTICLE ON AEROBIC BIODEGRADATION OF COMPLEX ORGANIC
 MIXTURES. (K)
 DUE: 12/30/86 REVISED: 04/30/87 COMPLETED: 04/30/87

7672 BOOK CHAPTER - ABIOTIC ORGANIC CHEMICAL TRANSFORMATIONS AT THE SEDIMENT
 PARTICLE-WATER INTERFACE. (K)
 DUE: 05/30/87 REVISED: 01/01/00 COMPLETED: 05/30/87

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY
ISSUE: 0 ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION
PPA (L): 10 TRANSPORT AND FATE PROCESS DETERMINATION

PPA (S): 10 TRANSPORT AND FATE
RC: K ERL ATHNS
PROJECT: 09 Process Characterization for Toxics (Chemical)
PROJECT OFFICER: Richard G. Zepp PHONE: FTS-250-3428

PLANNED START: 10/01/79 PLANNED END: 09/30/88

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## PROJECT DESCRIPTION:

GOAL: Characterize key chemical processes: direct-indirect photolysis, hydrolysis, redox reactions, and sorption/desorption and provide additional scientific understanding of sediment-water exchange to improve exposure and risk assessment models.

RATIONALE: The roles of inorganics in pollutant transformation by photolysis and the kinetics of redox reactions are inadequately understood for reliable use in exposure assessment models at the present time. These processes are known to be environmentally important in many cases.

APPROACH: Laboratory studies with natural waters, with sediments and with reference materials will be used as the basis for acceptance or rejection of proposed equations for the kinetics of transformation and equilibria of transformation processes. The laboratory studies will provide rates of equilibrium constants based on the models. Compounds and reaction conditions will be selected to permit generalizations about changes in molecular structure naturally occurring inorganic species; redox reactions of abiotic systems, ill e relative to biotic systems, will be studied.

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The interactions of photochemically produced iron(II) with hydrogen peroxide and resulting organic oxidations were studied during the quarter. Using anisole and nitrobenzene as chemical probes and octanol or formate ion as scavengers, we found that the yield of hydroxyl radicals from Fe(II)/hydrogen peroxide was found to be 40% at pH 6.2. A promising technique was developed for the direct simultaneous analysis of Fe(III) and Fe(II) in natural waters. Dr. Richard Zepp is stationed for the summer at the EAWAG Laboratory in Switzerland, studying photochemical processes with Swiss scientists.

Nitrobenzene reduction studies were extended to soil-water samples obtained from two aquifers. The disappearance rate constants were approximately five times slower in the aquifer samples than in sediment samples collected in

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

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the Athens area. Detailed concentration studies of substituted nitrobenzenes indicated that the disappearance rate constants were dependent on the initial concentration of the nitrobenzene derivative. Additional studies are in progress to determine the rate limiting step of the reduction process.

Redox studies were performed on two carbamate pesticides, Protham and Carbaryl, in an anaerobic sediment/water system containing 10% solids. Kinetic results are being interpreted; decay products of these two pesticides will be analyzed. In addition to these redox studies, the hydrolysis of chlorinated organic compounds is currently being investigated.

Studies of the degradation of synthetic dyestuffs in anaerobic sediments continue. The effects of pH on the distribution and kinetics of reduction were studied for a nonionizable dye, azobenzene, and an ionizable dye, Congo Red. Results indicate that pH will have little effect on the distribution and reduction of azo dyes containing non-ionizable functional groups. For those dyes that do contain ionizable groups, pH will play an important role in their distribution and, thus, transport in natural systems. Changes in pH, however, may have little effect on the rate of reduction of these dyes at the sediment-water surface.

Studies on sorption of ionizable organic compounds to soils, sediments and aquifer material continue. Experimental work confirms that partitioning of the anion of pentachlorophenol (pentachlorophenolate) between octanol and water is highly dependent on ionic strength of the water phase and that partitioning of both the ion-paired phenolate and free phenolate species into octanol is important.

A workshop entitled "Oxidation-Reduction Processes in Sediment/Water/Aquifer Systems" was sponsored by ERL-Athens at Estes Park, CO, April 28-30, 1987. A workshop on the Environmental Chemistry of Dyes, organized by the Athens Laboratory, has been tentatively scheduled for November 12-13, 1987, in Pensacola, FL. A symposium entitled "Environmental Chemistry of Ionic Xenobiotics," also organized by the Athens Laboratory, will be held at the SETAC conference in November.

A journal article entitled "Effects of Humic Substances on Analysis for Hydrogen Peroxide using Peroxidase-Catalyzed Oxidations of Triarylmethanes or p-Hydroxyphenylacetic Acid" (7683A) was delivered to OTS and submitted to Environ. Technol. Letters.

## SCHEDULE AND STATUS OF DELIVERABLES:

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7683 JOURNAL ARTICLE ON OXIDATION PROCESSES IN AQUATIC ENVIRONMENTS. (K)
DUE: 06/30/87 REVISED: 01/01/00 COMPLETED: 06/30/87

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CODE TITLE  
BUDGET SUB-ACTIVITY: L104 TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY  
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION  
PPA (L): 10 TRANSPORT AND FATE PROCESS DETERMINATION  
PPA (S): 10 TRANSPORT AND FATE  
RC: K ERL ATHNS  
PROJECT: 37 Microbial Transformation Rate Constants  
PROJECT OFFICER: William C. Steen PHONE: FTS-250-3776  
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PLANNED START: 10/01/85 PLANNED END: 12/31/99  
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## PROJECT DESCRIPTION:

GOAL: Develop and apply decision-tree protocols for measuring microbial transformation rate constants for use in exposure and risk assessment models.  
RATIONALE: Scientifically valid and accurate transformation rate constants are required as inputs to mathematical models and other decision tools to assess risk associated with toxic chemicals in the environment.  
APPROACH: Laboratory studies will be conducted to define the critical variables and adapt or devise effective techniques for measuring microbial transformation rate constants. Decision-tree protocols will be developed and tested to delineate the steps and options to be exercised in such measurements. Protocols will be applied to selected toxic chemicals of critical interest.

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Following investigations with the seven chemicals reported during the last quarter, several areas surfaced warranting further study. The first activity was to investigate differences observed in second-order rate constants with microorganisms from the oxidation pond and from Hickory Hill aquatic systems. As a result of the approximate 3 orders of magnitude difference in calculated constants for the 4-dimethyl amino phenethyl alcohol in the oxidation pond versus Hickory Hill pond, i.e.  $(2.14 \pm \text{or} - 1.73) \times 10^{-11}$  and  $(1.96 \pm \text{or} - 1.67) \times 10^{-8}$  L per org. per hour, respectively, all seven chemicals are being re-investigated in the Hickory Hill pond water. To obtain measurable rates of transformation, it has been necessary to concentrate organisms from the Hickory Hill pond followed by resuspension to increase the initial population densities such that slowly degraded chemicals such as Alachlor, Propachlor, and Pronamide could be measured in the Hickory Hill site. Samples of Hickory Hill pond (approx. 20 L) were transported to the laboratory for filtration (millipore) in order to concentrate bacterial populations (10:1). Resulting filters were resuspended in appropriate volumes of pond water and shaken on the gyratory shaker for 48 hours. Following division of the bulk sample to reaction flasks, Alachlor was

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ERL ATHNS: APRIL - JUNE 1987

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:  
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spiked to desired concentrations. Initial plate counts of bacterial densities indicated the concentration steps had been successful. Bacterial densities were proportionately one order of magnitude higher, as was expected.

Although first attempts to concentrate were successful, Alachlor transformation appeared substantially slower than anticipated. The experimental investigation was reestablished for both Alachlor and Monalide. Alachlor results are being analyzed and appear to exhibit a preliminary rate constant of approximately  $10^{-13}$  L per org. per hour. Monalide experiments have just been initiated at time of reporting. Two more experiments measuring temporal variation of the methyl esters of 2,4-dichlorophenoxyacetic acid rate constant were completed. Results are consistent with the other 2,4-DME studies.

Good correlation was found to support the theory that the same structural features are responsible for infrared spectra and rates of compound degradation. Results correlating spectral data with both hydrolysis and biolysis rate constants for phthalate esters are being prepared as a journal article. A related study on biolysis of secondary amides has begun.

Dr. Tim Collette presented a poster session entitled "Correlation of Infrared Spectroscopic Data with Degradation Rate Constants" at the 17th Annual Symposium on the Analytical Chemistry of Pollutants, May 18-20, at Jekyll Island, GA.

## SCHEDULE AND STATUS OF DELIVERABLES:

# 6930 Interim Protocol for Measuring Microbial Transformation Rate Constants for Suspended Populations  
DUE: 11/30/87 REVISED: 01/01/00 COMPLETED: 01/01/00  
# 7282 REPORT ON MICROBIAL TRANSFORMATION RATE CONSTANTS FOR SUSPENDED POPULATIONS  
DUE: 03/30/87 REVISED: 12/31/87 COMPLETED: 01/01/00

CLIENT OFFICE:

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH  
ERL ATHNS: APRIL - JUNE 1987

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION
PPA (L): 11 EVALUATION OF EXPOSURE ASSESSMENT METHODS

PPA (S): 11 MICROCOSM/FIELD
RC: K ERL ATHNS
PROJECT: Q5 Protocols for Chemical Transformation Rate Constants
PROJECT OFFICER: Jackson Ellington PHONE: FTS-250-3197

PLANNED START: 10/01/83 PLANNED END: 12/31/99

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## PROJECT DESCRIPTION:

GOAL: Develop and apply decision-tree protocols for measuring chemical transformation rate constants and partition coefficients for use in exposure and risk assessment models.

RATIONALE: Scientifically valid and accurate transformation rate constants and partition coefficients are required as inputs to mathematical models and other decision tools to assess risk associated with toxic chemicals. Risk assessments are necessary in PMN and retrospective evaluations of toxic chemicals in the environment.

APPROACH: Laboratory studies will be conducted to define the critical variables and adapt or devise effective techniques for measuring chemical transformation rate constants and partition coefficients. Decision-tree protocols will be developed and tested to delineate the steps and options to be exercised in such measurements. Protocols will be applied to standard reference compounds for evaluation of accuracy and precision and to selected toxic chemicals critical interest.

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The Coordinated List of Chemicals, which identifies chemicals being regulated or studied by EPA, has been stored in a computerized database. The EPA/ATSDR Rank Superfund Hazardous Substances List has been added to the database collection of lists. This list is a joint action by EPA and the Agency for Toxic Substances and Disease Registry (ATSDR) and identifies the 100 most commonly found hazardous substances at Superfund sites. The substances are ranked within the list, according to the degree to which each poses a potential human health risk. Participation in the Coordinated List of Chemicals project has been solicited from all ORD laboratories (with five positive responses received to date). The information retrievable from the database will reveal who is studying what in ORD and stimulate communication among researchers, facilitate selection of chemicals for study (since practically all chemicals listed are of interest to the Agency), and permit Program Offices to obtain information on

continued...

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

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chemicals right when they become available and not months or years later when data are published.

William Donaldson presented a paper entitled "Constants for Predicting the Fate of Chemicals in the Ambient Environment" at the 17th Annual Symposium on the Analytical Chemistry of Pollutants, May 18-20, at Jekyll Island, Georgia.

The evaluation criteria for the database of physical, chemical, and microbial rate and equilibrium constants have been reviewed by ERL-Athens scientists. The criteria, which will be used to evaluate the reliability (quality) of literature data, have been compiled into a document that will be submitted for publication. Evaluation criteria were developed for 12 parameters.

## SCHEDULE AND STATUS OF DELIVERABLES:

# 7710 Interim Protocol for Measurement of Hydrolysis Rate Constants  
DUE: 03/31/88 REVISED: 01/01/00 COMPLETED: 01/01/00

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ERL ATHNS: APRIL - JUNE 1987

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION
PPA (L): 11 EVALUATION OF EXPOSURE ASSESSMENT METHODS

PPA (S): 11 MICROCOSM/FIELD
RC: K ERL ATHNS
PROJECT: 16 Evaluation of Exposure Assessment Methods
PROJECT OFFICER: Harvey W. Holm PHONE: FTS-250-3103

PLANNED START: 10/01/79 PLANNED END: 09/30/88

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## PROJECT DESCRIPTION:

GOAL: Develop and apply laboratory and field systems for testing transport and transformation subroutines, exposure modeling systems, and risk analysis systems.

RATIONALE: Methodologies for predicting and/or assessing ecological hazards have not been adequately tested in complex microcosm and field studies.

APPROACH: The use of controlled laboratory ecosystems to evaluate exposure modeling systems and risk analysis systems increases the probability of attributing a testing mismatch to the appropriate subroutine. To evaluate general applicability, microcosm results are compared with field data. Field and laboratory ecosystems having different physical, chemical, and biological makeup are developed and used for testing mathematical methods for determining eco-structure, evaluating ecological hypotheses and modeling assumptions used for developing generalized predictive models, and testing exposure assessment and risk assessment models.

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A manuscript (7618A), "Biogeochemical Cycling of Organic Matter in Acidic Environments: Are Microbial Degradative Processes Adapted to Low pH?" (Benner, Lewis, Hodson) has been cleared for publication in a CRC series, "Microbial Interactions in Acid Stressed Aquatic Ecosystems" (S.S. Rao, ed.).

A computer model for EXAMS has been written that incorporates research concerning predicting attached microbial transformation rates and their relative contributions to suspended organisms. Dr. Holm is field testing the model while on a sabbatical at Montana State University during the summer of 1987.

The journal article, "Effects of hardness, alkalinity, and pH on the toxicity of pentachlorophenol to *Selenastrum capricornutum*, Printz," has been modified in response to reviewer comments and accepted for publication by Environmental Toxicology and Chemistry (Smith, Brockway, Stancil) (7284C).

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

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Work has begun on systems in which to expose fish to continuously flowing, constant concentrations of toxicants to study chemical activity in the blood of fish at time of death.

## SCHEDULE AND STATUS OF DELIVERABLES:

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7618 JOUR. ART. ON ENVIRONMENTAL FACTORS AFFECTING MICROBIAL TRANSFORMATION
 RATES OF POLLUTANTS (K)
 DUE: 08/30/87 REVISED: 01/01/00 COMPLETED: 04/30/87

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 ERL ATHNS: APRIL - JUNE 1987

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CODE TITLE
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BUDGET SUB-ACTIVITY: L104 TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY
ISSUE: 6 STRUCTURE ACTIVITY RELATIONSHIPS
PPA (L): 20 STRUCTURE ACTIVITY RELATIONSHIPS AND ESTIMATION

PPA (S): 20 SAR/EST TECHNIQUES
RC: K ERL ATHNS
PROJECT: 10 Predictive Methods for Environmental Exposure Assessments
PROJECT OFFICER: Samuel W. Karickhoff PHONE: FTS-250-3149

PLANNED START: 10/01/80 PLANNED END: 09/30/88

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## PROJECT DESCRIPTION:

GOAL: Develop and test concepts for predicting key environmental transport, transformation and distribution processes for exposure and risk assessments of toxics.

RATIONALE: Computational procedures are needed for estimation of photochemical, hydrolytic and other transformation rates used in exposure assessments. Such computational approaches minimize the amount of measurement required and provide the only independent assessment of measured values.

APPROACH: Conceptual relationships and equations relating light absorption and rate constants to molecular structure will be developed for direct photolytic and hydrolytic transformation. Process rate constants and equilibrium constants will then be measured in the laboratory using natural components. Resulting data will be used to evaluate and/or modify the concepts and resulting equations.

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Approximately 15,000 ionization constants for pKa and pKb have been collected from the literature and cataloged. A pK database has been designed for input of the constants. This will be used to test the reliability of the computational algorithm for predicting values of pKa and pKb. The algorithm for computing pK has been written in Prolog.

An additional 680 UV absorption spectra have been digitized and added to the spectral database. This database will be used for calibration of computational algorithms and validation of the expert system's predictive capability for photochemical rate constants. The scheme for computing steric effects of substituent groups at two levels distant from the center or mass of the molecule was implemented.

Work continues to: 1) develop a second molecular orbital computational scheme suited for non-alternate organic compounds, 2) extend structural query

continued...

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

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and spectral computational schemes to compounds having three or four condensed rings, and 3) evaluate software and modify the code for graphic input of molecular structure into SPARC.

## SCHEDULE AND STATUS OF DELIVERABLES:

# 6929 JOURNAL ARTICLE ON ESTIMATING pKa's OF ORGANIC ACIDS AND BASES  
 DUE: 03/31/87 REVISED: 04/30/88 COMPLETED: 01/01/00

CLIENT OFFICE:

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ERL ATHNS: APRIL - JUNE 1987

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY
ISSUE: 6 STRUCTURE ACTIVITY RELATIONSHIPS
PPA (L): 20 STRUCTURE ACTIVITY RELATIONSHIPS AND ESTIMATION

PPA (S): 20 SAR/EST TECHNIQUES
RC: K ERL ATHNS
PROJECT: 15 PRC Relationships and Other Estimation Techniques
PROJECT OFFICER: Harvey W. Holm PHONE: FTS-250-3103

PLANNED START: 05/01/83 PLANNED END: 09/30/89

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## PROJECT DESCRIPTION:

GOAL: Expand data bases for establishing Property Reactivity Correlations (PRC) and develop quantitative relationships between microbial rate constants and molecular descriptions.

RATIONALE: There is a need for developing predictive models for fate and effects based on SAR/PRC, because resource limitations preclude laboratory characterization of all chemicals of interest.

APPROACH: Lab studies with natural water samples will be used as a basis for assessing formulations for the kinetics of processes describing microbial transformation of pesticides and other toxic chemicals. Emphasis will be placed on measurements of biomass associated with transformations. A homologous series of compounds will be used to examine how systematic changes in compound structure influence the microbial rate constants. Product analyses will be used to verify common transformation mechanisms.

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Dr. Benner made two oral presentations: (1) "Microbial transformations and fate of particulate organic matter in estuarine waters and sediments" at the Chesapeake Biological Laboratory, University of Maryland, and (2) "Depletion of <sup>13</sup>C in lignin: Implications for stable carbon isotope studies," at the Marine Biological Laboratory, Woods Hole, MA. He also participated in an EPA-sponsored workshop "Oxidation-reduction processes in sediment/water/aquifer systems" at Estes Park, CO, and an NSF-sponsored workshop "Stable isotopes as natural tracers in ecosystems, Woods Hole, MA. Laboratory experiments were begun to compare several estimates of bacterial biomass (microscopic direct counts, MPN determinations, agar plate counts) for use in second-order rate equations to predict the transformation rates of xenobiotics (phenol and p-cresol) in natural waters. John Barnett, technical assistant, has been trained to carry out these studies, which should be concluded in September 1987.

## SCHEDULE AND STATUS OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY
ISSUE: 1 ECOLOGY: ECOTOXICITY AND RISK ASSESSMENT
PPA (L): 26 DEVELOP METHODOLOGIES FOR ECOLOGICAL RISK ASSESSMENT

PPA (S): 26 RISK ASSESSMENT DEV.
RC: K ERL ATHNS
PROJECT: 13 Predictive Techniques for Ecological Risk
PROJECT OFFICER: Ray R. Lassiter PHONE: FTS-250-3501

PLANNED START: 10/01/84 PLANNED END: 09/30/90

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## PROJECT DESCRIPTION:

GOAL: Develop modeling approaches for assessment of risk from toxic chemicals in natural systems.

RATIONALE: Assessing risk from toxic chemicals involves assessments of concentration distributions in the environment and of expected effects.

APPROACH: Exposure analysis models will be used to provide expected aquatic environmental concentration distributions. To develop the capability to analyze for expected effects, it will be necessary, first, to determine what effects are of concern (population, community, ecosystem), and the appropriate aquatic systems to use to study those effects, then to develop the appropriate models to represent effects at those levels. Models for effects are adapted from existing models or developed on basic principles, as required. Finally, exposure analysis models are linked in a computer implementation with effects models via a user-friendly interface to provide the working risk analysis modeling system.

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

## Exchange Model

The paper, "Kinetic exchange of nonpolar organic chemicals by fish (Barber, Suarez, Lassiter) has been revised and will be resubmitted to Environmental Toxicology and Chemistry as a new manuscript. An important addition to the paper is an analysis of the gill uptake efficiency studies of Dr. Jim McKim, ERL-Duluth. In particular, predicted extraction efficiencies of the GETS model agree qualitatively with McKim's findings, regarding their dependence on logP. GETS was successfully coupled to the exposure models EXAMS and TOXIWASP and was presented at a workshop at EPA Headquarters in May. GETS was updated to simulate bioaccumulation of toxicants under dynamic exposure scenarios, and now will simulate bioaccumulation for constant, sinusoidal, exponential or arbitrary water concentrations. A joint food or gill exchange model, FORGETS, is being developed and will be available for the exposure workshop to be held in Athens.

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:  
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in August.

A fully automated respirometer for swimming fishes in which definitive studies of oxygen and toxicant uptake will be performed has been completed under the Montana State University cooperative agreement with subcontract to the University of British Columbia, and preliminary tests have been conducted.

Plant Uptake Studies

Studies were completed for two species of aquatic plants to determine their uptake characteristics for d1- and tetrachlorobenzene. Equilibrium with the water is reached for dichlorobenzene within 3 days, but tetrachlorobenzene does not saturate within 20 days. A model for chemical exchange between plant and water was developed and is being tested against the experimental data.

Derivation of the plant toxicokinetic model and its implementation in MathCAD code was followed by exploratory use of the model and comparison of model output to experimental data.

Population Effects Model

First draft manuscripts describing the individual growth model component of the population effects model and the static population effects analysis were completed. A population model using a "family tree" algorithm has been completed for testing and further development. Early results show promise of real benefits for use in risk assessment. Model results permit prediction of effect on population density followed by recovery of the population after cessation of exposure. Multiple exposures as well as time varying exposures are possible. A partial differential equation representation of population response was formulated, and work begun at the University of Tennessee to implement this in a working computer program. Description of the population model and its component individual-level models were included in the workshop given in Washington to update the program office personnel on the capabilities for risk assessment being developed in our research program. The population model coding was completed.

Development of Biota Database for Risk Assessment

An ecotoxic assessment database users and developers group was formed. During the last EcoRisk all-investigators' meeting (March 1987), the need for better communications was recognized and each member supplied a short description of the database(s) under his/her control. This information was compiled and distributed among the members. The list will be updated approximately every 6 months.

Lead Laboratory Review and Coordination for the EcoRisk Program

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The SAB review panel made its presentation to Assistant Administrator Barnes on April 21 following which the final draft response document was transmitted to OEPER Headquarters for processing. The OEPER quarterly report was conducted via a public seminar (OPTS Exposure Assessment Seminar Series) and a 3-day workshop to introduce program office analysts to EcoRisk products and software.

Five new deliverables were identified in response to needs of OPTS for short-term products on specified, agreed-on topics. Other activities this quarter have focused on development of materials for an FY88 work plan, progress report, and fiscal report; written response to the March peer review panel; and improving visibility and communications of the EcoRisk Program with program offices and EcoRisk coordinators and investigators.

SCHEDULE AND STATUS OF DELIVERABLES:  
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- # 7495 Documentation Report on Databases to Support Aquatic Ecosystem Models  
DUE: 08/31/87 REVISED: 01/01/90 COMPLETED: 01/01/90
- # 7505 Computer Program of Model Predicting Kinetic Exchange of Hydrophobic Xenobiotics  
DUE: 09/30/87 REVISED: 01/01/90 COMPLETED: 01/01/90
- # 7507 JOURNAL ARTICLE TESTING THE MODEL ASSUMPTION OF A SINGLE LETHAL CHEMICAL ACTIVITY FOR A SPECIES FOR NEUTRAL HYDROPHOBIC CHEMICALS  
DUE: 07/31/88 REVISED: 11/30/89 COMPLETED: 01/01/90
- # 7508 Prototype Population Model and Software Incorporating Lethal Effects of Narcotic Chemicals on Natural Populations  
DUE: 09/30/86 REVISED: 08/31/87 COMPLETED: 01/01/90
- # 7510 POPULATION MODEL AND SOFTWARE INCORPORATING LETHAL AND NONLETHAL EFFECTS ON FEEDING BEHAVIOR FOR CHEMICALS THAT ACT BY REVERSIBLE MODES OF ACTION  
DUE: 08/31/88 REVISED: 08/31/90 COMPLETED: 01/01/90
- # 7511 JA on Relevance of Sublethal Effects for Ecological Prediction  
DUE: 07/31/89 REVISED: 01/01/90 COMPLETED: 01/01/90
- # 7512 DOCUMENTATION REPORT ON SPECIFICATIONS FOR INPUT PARAMETERS AND COMPUTER CODE FOR AQUATIC ECOSYSTEM MODELS  
DUE: 08/31/88 REVISED: 08/31/90 COMPLETED: 01/01/90
- # 7513 COMPUTER CODE FOR FIRST OPERATIONAL VERSION OF AN ECOLOGICAL EFFECTS MODEL FOR AQUATIC ECOSYSTEMS  
DUE: 08/31/90 REVISED: 08/31/92 COMPLETED: 01/01/90

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SCHEDULE AND STATUS OF DELIVERABLES:

# 7514 REPORT ON STATISTICAL ANALYSIS OF TESTS OF ECOSYSTEM MODEL  
 DUE: 08/31/91 REVISED: 08/31/93 COMPLETED: 01/01/00

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| CODE                               | TITLE                                                |
|------------------------------------|------------------------------------------------------|
| BUDGET SUB-ACTIVITY: L104          | TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY        |
| ISSUE: I                           | ECOLOGY: ECOTOXICITY AND RISK ASSESSMENT             |
| PPA (L): 26                        | DEVELOP METHODOLOGIES FOR ECOLOGICAL RISK ASSESSMENT |
| PPA (S): 26                        | RISK ASSESSMENT DEV.                                 |
| RC: K                              | ERL ATHNS                                            |
| PROJECT: 28                        | Risk Assessment Methodologies for Toxic Substances   |
| PROJECT OFFICER: Robert B. Ambrose | PHONE: FTS-250-3160                                  |
| *****                              |                                                      |
| PLANNED START: 10/01/85            | PLANNED END: 12/31/99                                |
| *****                              |                                                      |

PROJECT DESCRIPTION:

GOAL: Develop computerized risk assessment system that helps OPTS analysts conduct various tiers of risk assessments efficiently, including methods for quantifying uncertainty in risk analyses, and procedures for optimal use of laboratory data, field studies, and modeling techniques.

RATIONALE: Risk assessment requires a wide variety of data and analysis techniques to implement the multi-tiered approaches used by OPTS. Efficient software can help OPTS analysts bring together appropriate data and analysis techniques in an appropriate structure for each specific risk assessment. Present exposure and effects models rarely give the estimates of uncertainty that are required to reduce total uncertainty while minimizing implementation cost.

APPROACH: A team will be assembled to review various types of risk assessment conducted by OPTS. Functional objectives will then be developed. Existing software be reviewed including GEMS and ANNIE. Relational data bases will be incorporating all submodels, databases and uncertainty analysis techniques. Protocols will be evaluated by laboratory and field studies to optimize risk assessment procedures.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A 3-day workshop entitled "Prototype Decision Support Software for Ecological Risk Assessment" was presented to OPTS staff. As part of the workshop, experts demonstrated the IRIMS Decision Support Software in EPA headquarters. The workshop was attended by many program office staff.

Sensitivity and uncertainty analyses are being used to compare error propagation in two different mathematical models of bioaccumulation of toxic substances. One approach uses thermodynamic concepts to describe chemical exchange; the other invokes a food chain approach.

An interagency agreement with the U.S. Bureau of Reclamation for develop-

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ment of a decision support system was initiated. This agreement enables a "translation" of the IRIMS system developed by IASA to the program goals of the EcoRisk research program.

SCHEDULE AND STATUS OF DELIVERABLES:  
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# 7493 Computer Program for Prototype Ecological Risk Assessment System  
DUE: 08/31/88 REVISED: 01/01/00 COMPLETED: 01/01/00

# 7496 Update WASP 4.1 Aquatic Exposure Model for Risk Assessment  
DUE: 09/30/87 REVISED: 01/01/00 COMPLETED: 01/01/00

# 7497 Update Stratified Lake Transport Model for Risk Assessment  
DUE: 09/30/88 REVISED: 09/30/89 COMPLETED: 01/01/00

# 7498 Sediment Transport Model for Risk Assessment  
DUE: 09/30/88 REVISED: 01/01/00 COMPLETED: 01/01/00

# 7499 General Bed-Water Exchange Model for Risk Assessment  
DUE: 09/30/88 REVISED: 09/30/89 COMPLETED: 01/01/00

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CODE TITLE  
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BUDGET SUB-ACTIVITY: L104 TOXIC CHEMICAL TESTING & ASSESSMENT NONENERGY  
ISSUE: J SUPPORT  
PPA (L): 30 TECHNICAL EVALUATION AND ASSESSMENT  
  
PPA (S): 30 TECHNICAL EVALUATION  
RC: K ERL ATHNS  
PROJECT: 31 Technical Evaluation and Assistance  
PROJECT OFFICER: Lee Mulkey PHONE: FTS-250-3160  
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PLANNED START: 10/01/79 PLANNED END: 12/31/99  
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PROJECT DESCRIPTION:  
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GOAL: Provide technical assistance to OTS and other program offices on complex problems relating to environmental exposures, system effects, hazards/risks, and benefit-risk assessments for toxic chemicals regulation and control.  
RATIONALE: OTS and other offices (e.g., OW, OPP, OSW and OPPE, Regions) engaged in toxic chemical regulations and assessments require technical assistance from ORD. This project will maintain the required inhouse and extramural expertise.  
APPROACH: Athens ERL staff will organize and participate in appropriate consultations, workshops, reviews, special projects, etc., in support of OTS and other Agency activities, including the review of TSCA documents, position papers, strategies, etc., as expertise and resources permit. Access to "on demand" inhouse expertise and assistance for OTS, Regions, States and other related office activities will also be provided via maintenance of appropriate contracts and liaison with CERL and other Agency support groups. Support, provided under this project, and assistance to "integrated toxics" projects will also be

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:  
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Technical information on exposure modeling activities was provided to Mr. Jack Gakstatter and Ms. Jean Parker, ORD Liaisons with Regions 3 and 10. Model and technical assistance provided to the two regions was reviewed. Exposure modeling courses and other training was described.

Paul Mitnik, State of Maine, was given technical information on stratified estuary application of WASP and MERGE, an ocean discharge model.

Wayne Davis, Water Monitoring Team, Region 5, was provided with technical information on exposure modeling. Mr. Davis recently joined Region 5 and will review exposure modeling efforts in the Region.

SCHEDULE AND STATUS OF DELIVERABLES:  
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## SCHEDULE AND STATUS OF DELIVERABLES:

# 7433 INTERNAL REPORT ON STATUS OF EXPOSURE & RISK MODELING  
SUPPORT PROVIDED BY CWQM TEAM  
DUE: 09/30/87 REVISED: 01/01/00 COMPLETED: 01/01/00

# 7649 INTERNAL REPORT ON STATUS OF CHEMICAL REVIEWS, ASSESSMENTS AND MODELING  
SUPPORT/TRAINING PROVIDED (K)  
DUE: 09/30/87 REVISED: 01/01/00 COMPLETED: 01/01/00

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| CODE                                          | TITLE                 |
|-----------------------------------------------|-----------------------|
| BUDGET SUB-ACTIVITY: R551                     | SUPPORT SERVICES-R&D  |
| ISSUE: A                                      | SUPPORT SERVICES, ORD |
| PPA (L): 01                                   | PROGRAM SUPPORT       |
| PPA (S): 01                                   | PROGRAM               |
| RC: K                                         | ERL ATHNS             |
| PROJECT: 32                                   | Support Services      |
| PROJECT OFFICER:                              | PHONE: FTS-250-3127   |
| *****                                         |                       |
| PLANNED START: 12/01/70 PLANNED END: 12/31/99 |                       |
| *****                                         |                       |

## PROJECT DESCRIPTION:

GOAL: Provide the non-personnel support services needed to operate OEPER/ORD's Athens Environmental Research Laboratory. The services include, but are not limited to, utilities, janitorial, guard services, facilities operation, and maintenance contracts.

RATIONALE: The services are required to keep Athens Environmental Research Laboratory operating.

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

NO PROJECT STATUS TEXT AVAILABLE

## SCHEDULE AND STATUS OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT



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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH  
ERL ATHNS: APRIL - JUNE 1987

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CODE TITLE

BUDGET SUB-ACTIVITY: Y105 HAZARDOUS SUBSTANCES NON-ENERGY
ISSUE: F PROVIDE TECHNICAL SUPPORT TO ENFORCEMENT, PROGRAM f REGIONS
PPA (L): 22 Enforcement and Other Technical Support/EPE
PPA (S): 22 Technical Support
RC: K ERL ATHNS
PROJECT: 04 Enforcement and Other Technical Support/EPE
PROJECT OFFICER: Harvey W. Holm PHONE: 8-250-3134

PLANNED START: 03/30/87 PLANNED END: 12/30/89

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## PROJECT DESCRIPTION:

GOAL: To provide Reg. technical support, expert advice, and new methods to conduct exposure/risk assessments for CERCLA sites. Emphasis is on the hazard ranking process and subsequent RIFS analysis. RATIONALE: Exposure assessment and fate/transport models, automated databases for soil, chemical biological and meteorological properties, and process transformation descriptions are under development or completed. Application and transfer of such technology to CERCLA ranking/assessment procedures/protocols have been limited. Working with Region 4/ATSDR will permit immediate application of improved methods, identify knowledge gaps, allow a focused study of exposure, health and environmental assessments. APPROACH: AERL, the Regions, via Region 4, and ATSDR will identify opportunities for joint technical activities, and demonstrate improved exposure and risk assessments. Case studies will be conducted including application of existing rank methods (HRS), mathematical models (multimedia analyses), and ecological risk procedures. Results will be compared to for additional research in fate/transport and exposure/risk assessment, and provide a basis

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

An exposure assessment workshop was developed for presentation to Regional and Headquarters staff and management engaged in exposure and risk assessment. Emphasis in the first of a series of four planned workshops will be water-related exposure. Dates are August 11-13, 1987, in Athens, GA. Attendees will receive operational versions of computer models and handbooks for conducting exposure assessments.

A technical review and modeling assessment was completed April 27, 1987, for a Region IV investigation of remedial actions at a disposal site in Florida. The rates of movement in soils for ethyl-4,4'-dichlorobenzilate, 4,4'-dichloro-alpha-trichloromethylene hydrol, DDT, DDE, and chromium were modeled as part of the basis for recommending appropriate remedial actions.

continued...

CLIENT OFFICE:

THIRD QUARTER STATUS REPORT ON FY'87 PROJECT DESCRIPTIONS  
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH  
ERL ATHNS: APRIL - JUNE 1987

## PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Reviews and discussions on the role of ecological assessments in initial hazard ranking for potential National Priority List sites were held with Regional and Headquarters staff. A work plan has been developed to investigate approaches for more comprehensive ecological risk assessments consistent with NPL ranking.

An Interagency Agreement with the U.S. Bureau of Reclamation for the development of decision support systems for ecological risk assessment was initiated. This agreement will produce a computer-based system to combine loading, exposure, and effects data/models for efficient, multimedia analysis of pollutant release, fate, and effects.

A cooperative agreement to characterize and define interactions within a microbial community that affect anaerobic degradation processes is being negotiated with Dr. Lily Y. Young, New York University Medical Center.

## SCHEDULE AND STATUS OF DELIVERABLES:

# 7772 Report on technical support to Regions for multimedia exposure assessments related to remedial actions.  
DUE: 11/30/87 REVISED: 01/01/00 COMPLETED: 01/01/00