

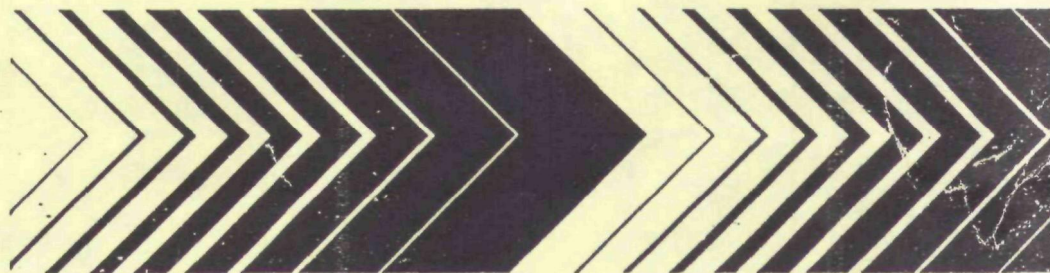
United States
Environmental Protection
Agency

July-September
1988

Research and Development

EPA Research Report

**Environmental
Research
Laboratory
Athens, GA 30613**



CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHMS: JULY - SEPTEMBER 1988

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CODE    TITLE
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BSA: B101 WATER QUALITY
ISSUE: A  WQBA/PERMITTING
PPA (L): 10 WASTELOAD ALLOCATION MODELING AND SUPPORT

PPA (S): 10 WASTELOAD ALLOCATION
RC: K      ERL ATHMS
PROJECT: 06 Environmental Process Characterization
PROJ OFFICER: Richard G. Zepp          PHONE: FTS-250-3428
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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 speciation and transport) 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.
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 conditions. Photochemical studies will emphasize the role of naturally 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 for metals with various solid substrates.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Studies on the role of trace metals in photochemical redox processes continue with work involving iron, copper and manganese. Two types of studies are being pursued involving iron. One is concerned with the effects of various environmental variables on the rate of oxidation and/or reduction of iron in aqueous solution. The reduction of iron(III) in the presence of fulvic acid was faster at higher pH, and the rate increased with irradiation at 436 nm. The second group of studies involves the degradation of several organic substrates exposed to sunlight in the presence of iron, hydrogen peroxide and octanol. In order of decreasing reactivity, the substrates examined were

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CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

p-nitrophenol, p-cresol, nitrobenzene, and atrazine. Other substrates will be tested using the same system.

The kinetics of the photochemical reduction of copper(II) to copper(I) have been studied in the presence of salicylate, chloride, or Tris. Salicylate and chloride had a small positive effect on the reaction rate; a more pronounced increase was observed with Tris, which complexes with the Cu(I) formed. The effects of other ligands on the rate of reaction will be examined.

Studies of the reactions of manganese oxides with phenols are continuing. Previous work indicated that the oxidation of several phenols by MnO₂ was enhanced by sunlight and that the reaction rates increased with decreasing pH. This quarter, the dark reactions of p-chlorophenol with MnO₂ at pH 4.2 were examined; the disappearance of p-chlorophenol was faster with Mn(IV) than with Mn(III). These experiments will be repeated using light.

Results of partitioning of 10 ionizable (anionic) organic compounds between water and octanol as a function of aqueous phase inorganic ion concentration and composition (LiCl, KCl, NaCl, CaCl₂, and MgCl₂) and pH are discussed in a manuscript currently in preparation. The relevance of this work to adsorption behavior (and hence, the ultimate fate and toxicity) of ionizable organic pollutants in the environment is addressed.

Laboratory work investigating sediment-organic anion interactions continues. Partition coefficients have now been measured for two anionic organic compounds (DNOC and silvex) in 12 well-characterized sediments. Although partitioning appears to be strongly influenced by hydrophobic interactions (as expressed by fraction of organic carbon), other system characteristics such as pH and conductivity (a measure of aqueous phase ionic strength) also may influence partitioning.

In earlier work at ERL-Athens, the reaction rate for anaerobic biolysis of para-substituted nitrobenzenes was observed to be slower with increasing chain length of the substituent. A good correlation could be made between reaction rate and Van der Waals radii. Results of current experiments show that this correlation does not hold with aliphatic para-substituted anilines. It appears that two distinct degradation pathways are functioning in this case--the first being biological attack on the aniline group and the second the biochemical oxidation of the aliphatic chain. Attempts are being made to isolate bacteria that degrade octylaniline and aniline in spiked natural water. If this succeeds, kinetic and product studies will be conducted with pure bacterial cultures to confirm the observation that two biological pathways were operating in the para-substituted aniline degradation.

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CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Dr. Eric Weber and Mr. George Baughman attended the EPA-sponsored Azo Dye and Pigment Regulatory Workshop in Raleigh, NC, on August 15-17, 1988. They presented their latest research findings and participated in discussions to develop a regulatory strategy for azo dyes. In support of this effort, samples from the influent and the effluent of a municipal treatment plant receiving waste from a North Carolina textile mill were analyzed. Thin layer chromatography indicated the presence of approximately 20 dyes in the influent and 3 dyes in the effluent. The dyes in the effluent are most likely acid or direct dyes. Methodology currently is being developed to separate and isolate the dyes in the effluent sample.

STATUS AND SCHEDULE OF DELIVERABLES:

8054 INTERNAL REPORT (RESEARCH BRIEF) ON PHOTOCHEMICAL DEGRADATION OF ORGANIC POLLUTANTS IN THE AQUATIC ENVIRONMENT
DUE: 07/31/88 REVISED: 01/01/90 COMPLETED: 07/31/88

CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: B101 WATER QUALITY
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.
PROJ 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:

"Laboratory Procedure for Determining Substrate Removal Rate Coefficients for Biofilms" has been submitted to the Journal of Microbiological Methods; and "Assessing Interactions of Organic Compounds During Biodegradation of Complex Waste Mixtures" has been accepted for publication by Environmental Toxicology and Chemistry. "Microbial Activities in Surface Films at the Sediment-Water Interface" was presented by Dr. Lewis at a symposium entitled "Transport and Transformation of Contaminants Near the Sediment-Water Interface" held in Narragansett, RI.

Field and laboratory studies are being conducted on the effects of diffusion limitation on the microbial ecology of nonturbulent habitats and the significance of these effects on microbially mediated processes, such as degradation of toxic chemicals and nutrient cycling.

STATUS AND SCHEDULE OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT

CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: B101 WATER QUALITY
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
PROJ 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) and exposure assessment models for conventional and toxic pollutants for streams, rivers, lakes, and estuaries and provide OW with guidance and user assistance through the Center for Exposure Assessment Modeling (CEAM).
RATIONALE: Water quality-based NPDES revisions, WLAs, AWT assessments, use-attainability activities, and BMP selection by OW, 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 CEAM to provide modeling packages/manuals/tapes and data bases on request, conducting training seminars and workshops as required, and providing hands-on user assistance as resources permit.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Two model training courses, in part to support waste load allocation studies, were held this quarter: "Exposure and Bioaccumulation of Toxicants in Surface Water," July 25-28, 1988, Washington, DC, and August 15-18, 1988, Boulder, CO. Approximately 50 individuals attended each course.

A feature article entitled "Simulation Models for Waste Load Allocation of Toxic Chemicals--A State of the Art Review" was published in the Journal of Water Pollution Control Federation's September issue.

Cooperative agreement researchers at Tufts University presented a paper
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CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

entitled "Effect of Correlated Inputs on DU Uncertainty" at the 1988 Joint CSCE-ASCE National Conference on Environmental Engineering, July 13-18, 1988, Vancouver, British Columbia, Canada.

Work continues on graphical presentation of uncertainty information. A clear and concise presentation format is critical to the use of this information by decision-makers. Also, investigation of the impact of assumption of various distributions (normal, log-normal, uniform) continues.

Significant technical support to waste load allocation studies was provided including:

- o Dr. Steve McCutcheon participated in the workshop, "Transport and Transformation of Contaminants Near the Sediment-Water Interface," at Narragansett, RI, August 29-31, 1988, at the request of EPA's Office of Exploratory Research.
- o Mr. Robert Ambrose assisted Mr. Dennis Long, URS, Inc., Columbus, OH, in conducting a combined sewer overflow study for the City of Columbus. The effects of overflow on metals contamination (acute toxicity) and nutrient/carbonaceous pollutants (eutrophication/DO depletion) of the Scioto River are under study. WASP4 will be used.
- o Assistance was provided to Lynn Kring, Wasteload Allocation Coordinator, Region VII, Kansas City, KS, on settling effluent limits for oil and grease. Recent work on modeling the fate of oily wastes in surface waters was used.
- o Assistance was provided to Mr. Joseph Marknis, Office of Water Enforcement and Permits, Office of Water, in reviewing a report entitled "Task Two Summary Reviews for Administrative and Technical Assistance in the Preparation of Storm User Reports to Congress."
- o Assistance was provided to Mr. Jerome L. Pitt, Water Management Division, Region VII, Kansas City, KS, in formulating MINTEQA2 modeling scenarios for estimating dissolved lead in drinking water originating from solder joints.
- o Modeling assistance was provided at a planning meeting between State of Nevada, Clark County, City of Las Vegas, and EPA Region IX for a water quality modeling study of Las Vegas Wash and Bay on Lake Mead (at the request of Region IX).
- o The CEAM Electronic Bulletin Board System (BBS) continues to be well

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CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
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ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

used in support of waste load allocation activities. One hundred thirty-nine new users registered in this quarter, making a total of 319 users. Seven hundred sixty-six calls were placed to the BBS this quarter. Twenty-six input datasets were uploaded from users for debugging by CEAM staff. The BBS was in active use 11% of the quarter.

- o The following waste load allocation models were distributed in the fourth quarter:

	PC	BBS	MAINFRAME
WASP4	74	3	4
SWMM3	38	1	4
HSPF9	62	0	3
QUAL2EUNCAS	91	3	6
DYNTOX	40	0	3
EXAMS11	54	1	4
EGETS	9	2	0

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CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

o Two Summary Reviews for Administrative and Technical Assistance in the
o Assistance was provided to Mr. Jerome L. Pitt, Water Management

o Assistance was provided to Mr. Jerome L. Pitt, Water Management
Division, Region VII, Kansas City, KS, in formulating MINTEQA2 modeling
101B23P.12B101B23P.13B101B23P.14B101B23Q.20B101B26N.29B101B26N.33B101B26N.

STATUS AND SCHEDULE OF DELIVERABLES:

7851 REPORT ON EXPERT ADVISOR FOR CORNIX MODEL
DUE: 07/31/88 REVISED: 07/31/89 COMPLETED: 01/01/00

CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: B101 WATER QUALITY
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)

PROJ 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 and application
projects and technology transfer workshops, and symposia, 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 and
microbiological 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:

L.C. Brown and Qian Song, "Effect of Correlated Inputs on DO Uncertainty,"
presented at and published in proceedings of 1988 Joint CSCE-ASCE National Con-
ference on Environmental Engineering, July 13-15, 1988, Vancouver, B.C.

A manuscript entitled, "Metal Interactions at Sulfide Mineral Surfaces:
Part II. Adsorption and Desorption of Lanthanum," by Y. Lin, G.W. Bailey, and
A.T. Lynch was completed for presentation at the International Symposium on
Environmental Life Elements and Health, November 1-5, 1988, Beijing, China. A
manuscript entitled "Metal Interactions at Sulfide Mineral Surfaces: Part III.
Affinities in Single and Multiple Ion Adsorption Reactions," by Y. Lin, G.W.
Bailey, and A.T. Lynch was completed for presentation in a poster session at the

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CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Beijing Symposium. The papers will be published in the Symposium proceedings.

An abstract entitled "Metal Interactions at Sulfide Mineral Surfaces: Part IV. Adsorption and Precipitation Reactions," by Y. Lin, G.W. Bailey and A.T. Lynch has been accepted for poster session presentation at the American Society of Agronomy national meeting, November 27-December 2, 1988 in Anaheim, California.

Information from the research of both Mr. Jin and Mr. Lin was used as part of an AERL internal report to the Office of Solid Waste entitled "The Speciation of Toxic Metals in the Aquatic Environment," February 1988.

Dr. Brown is participating in an application of QUAL2E-UNCAS in southern California. Work continues on graphical presentation of uncertainty information. It is felt that a clear and concise presentation format is critical to use of this information by decision-makers. Also, investigation of the impact of assumption of various distributions (normal, log-normal, uniform) continues. These topics will be the subject of an M.S. thesis to be completed by December 1988.

Drs. Rosemarie C. Russo and Ray R. Lassiter presented papers at the International Symposium on Fish Physiology, Fish Toxicology, and Fisheries Management. The Symposium was sponsored by EPA, PRC National Science Foundation, Zhongshan University, Institute of Hydrobiology of the Academy of Sciences of China, Canadian Society of Zoology, American Fisheries Society.

STATUS AND SCHEDULE OF DELIVERABLES:

7174 MAGNETIC TAPE OF SUMM III.4 INCLUDING CORRECTIONS AND
ENHANCEMENTS.
DUE: 12/31/87 REVISED: 01/01/00 COMPLETED: 12/31/87

CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: B101 WATER QUALITY
ISSUE: A WQBA/PERMITTING
PPA (L): 15 ARTIFICIAL INTELLIGENCE AND EXPERT SYSTEMS

PPA (S): 15 EXPERT SYSTEMS
RC: K ERL ATHNS
PROJECT: 08 Expert System for Prediction of Physical/Chemical Parameters
PROJ OFFICER: Samuel W. Karickhoff PHONE: FTS-250-3149

***** PLANNED START: 06/01/85 PLANNED END: 09/30/99 *****

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 the development of 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 within the molecular structure primary reactive units versus perturbative or noncontributing units; (2) develop rules for classifying and characterizing reactivity; and (3) develop data to 'calibrate' with regard to reactivity.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Two refinements are being made in SPARC, the ERL-Athens expert system for predicting chemical reactivity parameters:

1) Since the quality of computational output necessarily reflects the quality of calibration of parameters in any successful quantitative chemical model, a "self-training" algorithm called TRAIN has been developed for SPARC. The program takes a set of target model parameters (initial values plus any appropriate boundary values) together with a set of designated data and provides an optimized set of model parameters. TRAIN cycles through a Jacobian optimization procedure, then sets up and executes the specifics of optimization as requested

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CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

by the user.

2) A performance validity (PV) program module is being written to assure that all computational elements in SPARC are working at optimum by being subjected to a variety of compounds (about 100) that represent different types of molecular reactivity. The nature of these representative compounds is such that all types of computation in the system are checked for evidence of any "rippling" effect that might remain unnoticed in the system. The purpose of PV is to sustain the validity of program code and performance as the total system (SPARC) is being developed. This will enhance confidence in the system as algorithms for other chemical reactivity parameters (hydrolysis, Kow, redox, etc.) are being developed.

Coding and input of compound pKa's into the data base is continuing. To date, 3067 compounds have been entered.

STATUS AND SCHEDULE OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT

CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: B101 WATER QUALITY
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

PROJ 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 knowledge-based expert systems or 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. Workshops, seminars, and problem-specific consultation in knowledge engineering will be provided to other ORD offices/labs as appropriate.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Mr. Tom Barnwell presented expert systems for QUAL2E and CORMIX models at a Region VII workshop in Kansas City, KS, on September 22, 1988. The workshop reviewed the range of expert systems currently available and under development within EPA.

Work continues on improving the CORMIX expert system for evaluating near-field mixing from point source discharges. Translation from M.I. a \$5,000 development tool to VP-Expert, available for less than \$100, is nearly complete.

STATUS AND SCHEDULE OF DELIVERABLES:

7161 REPORT ON EXPERT SYSTEM FOR SINGLE-PORT DISCHARGES IN UNSTRATIFIED RECEIVING WATER BODIES
DUE: 03/31/87 REVISED: 03/31/88 COMPLETED: 03/31/88

CLIENT OFFICE: OWR5

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

STATUS AND SCHEDULE OF DELIVERABLES:

7851 REPORT ON EXPERT ADVISOR FOR QUALZE
DUE: 07/31/88 REVISED: 07/31/89 COMPLETED: 01/01/90

CLIENT OFFICE: AA OW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: B101 WATER QUALITY
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

PROJ OFFICER: Lawrence A. Burns PHONE: FTS-250-3511

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. 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 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 computer model that can be used by technical personnel and environmental decision makers as an objective tool for rational risk/benefit evaluations in specific wetland basins.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A report (7885A) on progress to date in a project by EPA and the Geological Survey to improve water quality simulation models by providing automated access to digital databases and remotely sensed data was provided to the Office of Wetland Protection. Wetlands Research was granted a brief no-cost extension to complete their final report. No further activities will be undertaken in this project.

STATUS AND SCHEDULE OF DELIVERABLES:

7854 PROGRESS REPORT ON FIELD AND MODELING RESEARCH ON NUTRIENT DYNAMICS
IN FRESHWATER WETLANDS
DUE: 06/30/88 REVISED: 01/01/90 COMPLETED: 06/30/88

CLIENT OFFICE: AA OW

FOURTH QUARTER STATUS REPORT ON FY:88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

STATUS AND SCHEDULE OF DELIVERABLES:

7800 REPORT ON WDMIS (WATERSHED DATA MANAGEMENT SYSTEM) LIBRARY OF
WATERSHED MASTER DATA AND GRAPHICS PROCESSING ROUTINES
DUE: 07/31/88 REVISED: 01/01/88 COMPLETED: 07/31/88

CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY:88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: B101 WATER QUALITY
ISSUE: C WASTE WATER TREATMENT TECHNOLOGY
PPA (L): 46 IDENT. 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
PROJ OFFICER: John M. McGuire PHONE: FTS-250-3185

PLANNED START: 10/01/82 PLANNED END: 09/30/90

PROJECT DESCRIPTION:

GOAL: This research will identify and determine distribution of unlisted chemicals in industrial wastewaters. Compounds identifiable by empirical mass spectra matching and those eluding identified 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 that elude identification by spectra matching will be identified by reanalysis of samples using multispectral techniques (low res. MS, electron impact MS, low res. chemical ionization MS, high res. MS, FTIR spec.). Computerized multi spectral interpretation approaches will be developed to improve efficiency.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The paper, "Role of Vibrational Spectroscopy at the Environmental Protection Agency's Environmental Research Laboratory in Athens, Georgia" by J.W. Collette, was published in Appl. Spectros. 42, 1139 (1988).

A new mass spectrometer system was purchased through the Invitation for Bid mechanism. Installation will begin in November. The ORD Scientific Equipment Committee authorized replacement of our two obsolete Varian mass spectrometers, and a procurement action for a new instrument was implemented. The contract was awarded to VG Analytical for the VG 70 SEQ hybrid sector/

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CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

quadrupole MS/MS system controlled by VAX 2000 workstations. The system is state-of-the-art and includes a high resolution stage capable of better than 1:50000 resolving power as well as a final collision and quadrupole section capable of 100 pg detection of certain MS/MS transitions.

A significant decision was made during the quarter to discontinue processing of GC/MS tapes from the Office of Water and from Superfund effective January 1989. This decision was made due to the need for extensive and major modifications to the software for which resources are not available. Study of the results from the industries processed for the Office of Water during the last year indicated that both GC-peak recognition and quantitation using the software developed in 1977 at ERL-Athens were poorer than those obtained using the dedicated computers of state-of-the-art GC/MS systems. It is believed that the source of this is the CLEAN algorithm, which is the most patched, complex, and least understood portion of the coding. It is the one that we understand the least. The mandated change from the INFORM database set up here in the late 1970s to the FOCUS database itself requires the service of all of our programmers through the end of the calendar year. We recommend reprogramming the tape programs from the start, incorporating the FOCUS database management system and the most-up-to-date peak recognition and quantitation algorithms, before processing more tapes. Funds are not available to do this. It is expected that reprogramming will introduce a 1-year to 2-year delay in the overall tape programs if they are reestablished.

As targets for confirmation analytes from the Office of Water tape re-analyses, the following tentatively identified compounds have been selected from the POTW and Organic industries: N,N-dimethyl formamide; 2-nitrophenol; o-xylene; p-xylene; 1,3-diethyl benzene; chlorobenzene; phenol; o-t-butyl phenol; 2'-(2-ethoxyethoxy)-ethanol (carbitol); diethylene glycol monobutyl ether (butyl carbitol); m-dichlorobenzene; dimethyl methylphosphonate; diethyl ethylphosphonate; triethyl phosphate; trimethyl phosphate; tris-(2-chloroethyl) phosphate; tris-(1,3-dichloro-isopropyl)phosphate; isopropyl benzene; benzaldehyde; dimethyltrisulfide; 2,2'-methylene bis-(6-t-butyl-4-methyl phenol); benzoquinone; 2-chloro-4-nitro-aniline; 1,12-dodecandiol; p-chloronitrobenzene; diphenyl amine; n-tetradecane; n-docosane; caffeine; oleic acid; palmitic acid; stearic acid; dodecanol-1; all cresol isomers; all dimethyl phenol isomers; naphthalene; biphenyl; 1,2,4-trimethyl benzene; benzoic acid; and dibutylphthalate. Extracts for the POTW targets are on hand, and extracts for the Organic samples have been requested from the ITH Sample Control Center. The confirmation work will be reported in the next quarter.

Following the redesign and fabrication of the alignment bracket for the MAGIC LC/MS interface mentioned last quarter, the unit was tested on the CH5-DF mass spectrometer. Although the instrumental sensitivity was good, performance of the interface was poor. Comparing all aspects of the hardware in use at the

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CLIENT OFFICE: OWRS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Georgia Institute of Technology and in our in-house test, we determined that the limiting factor was the two pumps used to remove the solvent from the LC effluent. These pumps had been used previously at ERL-Athens in conjunction with development of the moving belt interface on the Finnigan 3200 and 4515 instruments. Two new pumps were ordered, but were not received before the CH5-DF was shut down in preparation for its being surplused. The interface will be evaluated with the new pumps on the VG 70 SEQ when it has been installed; this will delay the test into the second quarter of FY89.

STATUS AND SCHEDULE OF DELIVERABLES:

7577 REPORT ON TAPE STUDY OF GC/MS RUNS ON POTW SAMPLES
DUE: 11/30/87 REVISED: 05/31/88 COMPLETED: 02/29/88

7579 REPORT ON MULTI SPECTRAL IDENTIFICATIONS OF MIS LIB COMPOUNDS. (K)
DUE: 12/30/88 REVISED: 11/30/89 COMPLETED: 01/01/00

CLIENT OFFICE: ODW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: C104 DRINKING WATER
ISSUE: F GROUNDWATER
PPA (L): 62 Ground Water Methods, Information Transfer & Applications

PPA (S): 82 GW MTHDS, INFO, & APPL
RC: K ERL ATHNS
PROJECT: 22 Identify Unlisted Contaminants in Potential DW Sources
PROJ OFFICER: John McGuire PHONE: FIS-250-3185

PLANNED START: 10/01/87 PLANNED END: 12/31/99

PROJECT DESCRIPTION:

GOAL: Identify and determine frequency of occurrence of unlisted compounds that may pose a hazard to human health in potential drinking water sources with emphasis on potential groundwater contamination so that the contaminants can be prioritized for health assessments.

RATIONALE: The 1986 Amendments to the Safe Drinking Water Act require that lists of Recommended Maximum Contaminant Levels (RMCL) and monitoring requirements be published January 1, 1988 and every three years following for previously unregulated contaminants in drinking water that pose a health risk. Most monitoring programs identify only currently regulated compounds, therefore reanalysis of monitoring raw data is needed to identify unregulated compounds as candidates for listing.

APPROACH: Computer programs will be used to search GC/MS raw data from analysis of groundwater and other potential DW sources for unregulated compounds. Mass spectra will be compared with library spectra for identification. Compounds that cannot be identified by spectra matching will be identified by reanalysis of samples using multispectral techniques (low resolution electron impact MS, high resolution MS, Fourier transform IR spectrometry, chemical ionization MS).

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Progress Report on Analysis of Chlorination Products in Water by J. M. McGuire, I. W. Collette, A. D. Thruston, Jr., T. L. Floyd, and W. Payne, was provided to the Office of Drinking Water.

Ether extracts from samples collected at a pilot plant using a new chlorination process were received with no obvious loss during shipping from the Water Engineering Research Laboratory. A GC/MS run was obtained on the finished sample, but the concentrations of most analytes appear to be too low for effective use of GC/FTIR. One GC peak that is present at a moderate level

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CLIENT OFFICE: ODW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

corresponds to one of the unidentified, unchlorinated compounds in earlier WERL studies. It will be examined by GC/FTIR in early October.

STATUS AND SCHEDULE OF DELIVERABLES:

7810 Report on identification of unlisted chemicals for evaluation
as potential drinking water contaminants.
DUE: 08/31/88 REVISED: 01/01/00 COMPLETED: 08/31/88

CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
 OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
 ERL ATHNS: JULY - SEPTEMBER 1988

 CODE TITLE
 BSA: D109 HAZARDOUS WASTE
 ISSUE: C WASTE CHARACTERIZATION
 PPA (L): 26 LAND DISPOSAL ASSESSMENT & EVALUATION OF OTHER MGMT SYSTEMS
 PPA (S): 28 LAND DISPOSAL ASSESS
 RC: K ERL ATHNS
 PROJECT: 03 Measure Rate Constants and Partition Coefficients
 PROJ OFFICER: Jackson Ellington PHONE: FTS-250-3197

 PLANNED START: 10/01/85 PLANNED END: 12/31/99

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:

Products of hydrolysis were identified for 2,2-dichloropropane (CAS No. 594-20-7). A neutral rate constant of 4.1 (+/- 0.2)E-2 at pH 7 and 25°C was reported. The products determined by GC/MS analysis were acetone (CAS No. 67-64-1) and 2-chloropropane (CAS No. 557-98-2).

Preliminary results for 1,1-dichloroethane (CAS No. 75-34-3) indicated a half-life of more than 3 years at pH 7 and 25°C. The 1,1-dichloroethane degradation rate was significant because of its structural similarity to 2,2-dichloropropane and 1,1-dichloropropane, which are two chemicals of particular interest to OSW. Dr. Peter Jeffers, at ERL-Athens on an NRC appointment, is preparing a journal article that will include hydrolysis rate constants and activation energies for several di- and tri- substituted ethanes and propanes

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CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
 OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
 ERL ATHNS: JULY - SEPTEMBER 1988

 PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

 including the 1,1-dichloroethane. Jeffers' data and data previously generated at ERL-Athens can be compared to establish property reactivity correlations.
 Dr. Jackson Ellington spent approximately two weeks in August assisting Region III (Ruth Rzepski, Enforcement Project Manager) concerning hydrolysis of carbon disulfide and viscose rayon waste. He attended a meeting in Philadelphia on August 19 between Region III and Avtex Fibers personnel and co-authored an EPA Center for Exposure Assessment Modeling (CEAM) report that detailed the proposed fate of carbon disulfide and viscose rayon waste at the Avtex Fibers solid waste disposal facility.

In September, Mr. Valdas Jankauskas from the Lithuanian Soviet Socialist Republic visited the lab and received training in the measurement of hydrolysis rate constants using protocols developed by ERL-Athens. When he returns to his home lab, Mr. Jankauskas will measure second-order alkaline hydrolysis rate constants for six substituted acetanilides and provide the data to ERL-Athens. The hydrolysis rate data will be compared with infrared data for the six substituted anilides to test for property reactivity correlations for use in predicting hydrolysis rates. The amide bond is found in many chemicals of environmental interest in addition to the acetanilides.

Fate data for 44 chemicals and 24 transformation products that were submitted to OSW earlier were reviewed and verified for correctness for publication in the Federal Register pertaining to OSW's "concentration-based listing" program.

STATUS AND SCHEDULE OF DELIVERABLES:

- # 7950 Report on hydrolysis rate constants for enhancing property-reactivity correlations.
 DUE: 06/30/89 REVISED: 01/01/90 COMPLETED: 01/01/90
 # 7953 Third report on partition coefficients for land disposal assessment.
 DUE: 04/30/88 REVISED: 01/01/90 COMPLETED: 04/30/88

CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: D109 HAZARDOUS WASTE
ISSUE: C WASTE CHARACTERIZATION
PPA (L): 26 LAND DISPOSAL ASSESSMENT & EVALUATION OF OTHER MGMT SYSTEMS
PPA (S): 28 LAND DISPOSAL ASSESS
RC: K ERL ATHNS
PROJECT: 07 Environmental Process Characterization - Metals
PROJ OFFICER: Arthur W. Garrison PHONE: FTS-250-3145

PLANNED START: 10/01/84 PLANNED END: 12/31/99

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, especially MINTEQA.
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; metal-ligand structural studies will be conducted using laser 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 concerning the pH dependent distribution behavior of Ag, As, Ba, Be, Cd, Cr, Cu, Hg, Ni, Pb, Sb, Se, Tl, and Zn under oxic conditions on aquifer material samples from New Jersey, Texas, and Utah sites continued. A cation exchange column pre-concentration procedure for the detection of cationic contaminants in groundwater is being developed. An internal report, "Sample Acquisition Program for Bench Scale Testing of MINTEQA1: Sample Manager's Report" was provided to the Office of Solid Waste. A second document, Acquisition and Analysis of Groundwater/Aquifer Samples: Current Technology and the Trade Off between Quality Assurance and Practical Considerations, was

continued...

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FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

submitted for publication.

QA/QC experiments using the ICP are continuing; specific areas of inquiry include: a) the effects of sodium on transition element emission intensities, b) linearity of emission intensities as a function of contaminant concentration in the parts-per-billion concentration range, and c) optimization of element specific ICP operating conditions with particular emphasis on matrix effects and spectral interferences.

Plans are being made and equipment ordered to provide an in-house sub-surface region sampling capability. In addition to the development of pre-concentration procedures, in-line monitoring equipment has been ordered and an attempt is being made to equip a mobile laboratory.

Work continues on a spectral library of the ultraviolet-visible spectra of major minerals found in soils and sediments. Band deconvolution and separation into separate "peaks" is being done by using the first, second and third derivatives of the major peaks.

Studies of metal interactions with bacteria continue at the University of Arkansas and the University of Guelph. Single metal ion reaction versus multiple metal reaction with four bacteria was evaluated at Arkansas for the metals Ag(I), Cd(II), Cu(II), and La(III). In all cases, both the amount of metal sorbed and the KD were lower in the 4-metal treatment than in the single metal ion treatment. The total amount of Ag(I) bound, however, was not greatly reduced by the presence of Cd(II), Cu(II), and La(III). There was a difference in metal sorption by bacterial species; *P. aeruginosa* was the most efficient binder of metals.

Electron microscopy and energy-dispersive analytical x-ray analyses (done at the University of Guelph) of the metal-treated bacteria indicated that Ag(I) may actually be precipitated as elemental Ag both in the cell wall and the cytoplasm, while La(III) is bound only at the cell wall.

The metal remobilization studies of Cu(II), Ag(I) and Cr(III) pre-sorbed on bacterial cell walls and cell-wall clays using five leaching agents were completed at the University of Guelph. Cr(III) is highly stable in the cell wall, clay and composite wall-clay system. The effectiveness of the leaching agents for desorbing Cr(III) is H+ = EDTA = fulvic acid < lysocyme < Ca(II). A no-cost extension of this cooperative agreement was requested and granted until June 30, 1989.

Lanthanide ion probe spectroscopy is being used to investigate metal binding with humic materials. Software development for instrument control and

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CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

data collection for the excimer-dye laser system to be used for this spectroscopy is almost completed. Installation of the Ramanor U1000 macrosampling device and complete spectrometer and microscope alignment by an Instrument SA engineer was completed in September.

STATUS AND SCHEDULE OF DELIVERABLES:

8052 INTERNAL REPORT ON SPECIATION AND FATE OF TOXIC METALS IN THE AQUATIC ENVIRONMENT
DUE: 06/30/88 REVISED: 01/01/00 COMPLETED: 06/30/88

CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: D109 HAZARDOUS WASTE
ISSUE: C WASTE CHARACTERIZATION
PPA (L): 28 LAND DISPOSAL ASSESSMENT & EVALUATION OF OTHER MGMT SYSTEMS

PPA (S): 28 LAND DISPOSAL ASSESS
RC: K ERL ATHNS
PROJECT: 17 Environmental Process Characterization (Biological)
PROJ OFFICER: John E. Rogers PHONE: FTS-250-3592

PLANNED START: 03/01/85 PLANNED END: 12/31/99

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 concepts. 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:

Our current research efforts center on determining the appropriate kinetic equations to describe the transformation or degradation of hazardous organic chemicals in the environment, determining the effect of different head space gasses on the rates of degradation of dichlorophenols by the standard assay procedure, and evaluating the temporal and seasonal variability of the degradation rates.

STATUS AND SCHEDULE 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

CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: D109 HAZARDOUS WASTE
ISSUE: C WASTE CHARACTERIZATION
PPA (L): 26 LAND DISPOSAL ASSESSMENT & EVALUATION OF OTHER MGMT SYSTEMS

PPA (S): 28 LAND DISPOSAL ASSESS
RC: K ERL ATHNS
PROJECT: 21 Multimedia Modeling with Uncertainty Analysis
PROJ OFFICER: Lee A. Mukey PHONE: FIS-250-3160

***** PLANNED START: 09/01/85 PLANNED END: 12/31/99 *****

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 characteristics will be taken initially from OSW files and updated as appropriate. Multimedia models capable of simulating both the engineering controls and post-closure performance will be developed for use in evaluating banning waiver requests.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Effort this quarter in direct support of the Office of Solid Waste's development of a new rule for waste characteristics included detailed response to public comments received from prior proposed regulations citing the use of modeling in setting regulatory thresholds. ORD and ORD-contractor staff convened in OSW September 14-20 to participate in a work session on describing how the models MULTIMED AND EPACML were developed and used in the regulatory application.

A series of modifications have been made to the MINTEQA2/PRODEFA2 codes

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FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

that facilitate modeling five simultaneous sorbent phases using the newly added diffuse layer sorption model algorithm option. These changes were necessary to accommodate the revised OSW land disposal modeling scenarios. A general revamp of the preprocessor code that promotes user acceptance of the speciation model also was completed. Early feedback concerning these enhancements has been excellent.

Dr. David S. Brown completed an IPA assignment at Oregon State University. Part of his effort there was devoted to defining groundwater redox environments. Findings indicate platinum electrode measurements are not reliable indicators of Eh because of interferences caused by platinum oxide surface coatings. Eh electrodes so affected are expected to respond to hydrogen ion activity rather than redox potential. The clear empirical relationships between groundwater Eh and pH measurements indicate that this artifact is an almost universal problem for studies reported in existing Eh literature.

Draft final reports completed this quarter include:

"Landfill Source Model - A Module for Use in Multimedia Analysis of Land Disposal of Hazardous Wastes"

"A Generic Monte Carlo Simulation Shell for Uncertainty Analysis of Contaminant Transport Models"

"Enhanced Methods for Characterizing Uncertainties in Computationally Intensive Models"

STATUS AND SCHEDULE OF DELIVERABLES:

7919 USERS MANUAL FOR SARAH 2
DUE: 05/31/88 REVISED: 01/01/00 COMPLETED: 05/31/88

CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: D109 HAZARDOUS WASTE
ISSUE: C WASTE CHARACTERIZATION
PPA (L): 28 LAND DISPOSAL ASSESSMENT & EVALUATION OF OTHER MGMT SYSTEMS

PPA (S): 28 LAND DISPOSAL ASSESS
RC: K ERL ATHNS
PROJECT: 38 Environmental Process Characterization - Organics
PROJ OFFICER: N. Lee Wolfe PHONE: FTS-250-3429

PLANNED START: 10/01/84 PLANNED END: 12/31/90

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, sorption, and other processes will be related and quantified.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Results of partitioning of ten ionizable (anionic) organic compounds between water and octanol as a function of aqueous phase inorganic ion concentration and composition (LiCl, KCl, NaCl, CaCl₂, and MgCl₂) and pH are discussed in a manuscript currently in preparation. The relevance of this work to adsorption behavior (and hence, the ultimate fate and toxicity) of ionizable organic pollutants in sediments and the subsurface environment is addressed.

Laboratory work investigating sediment-organic anion interactions continues. Partition coefficients have now been measured for two anionic organic compounds (DNOC and silvex) in 12 well-characterized sediments. Although partitioning appears to be strongly influenced by hydrophobic interactions (as expressed in fraction of organic carbon), other system characteris-

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FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
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ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

tics such as pH and conductivity (a measure of aqueous phase ionic strength) also may influence partitioning.

In earlier work at ERL-Athens, the reaction rate for anaerobic biolysis of para-substituted nitrobenzenes was observed to be slower with increasing chain length of the substituent. A good correlation could be made between reaction rate and Van der Waals radii. Results of current experiments show that this correlation does not hold with aliphatic para-substituted anilines. It appears that two distinct degradation pathways are functioning in this case--the first being biological attack on the aniline group and the second the biochemical oxidation of the aliphatic chain. Attempts are being made to isolate bacteria that degrade octylaniline and aniline in spiked natural water. If this succeeds, kinetic and product studies will be conducted with pure bacterial cultures to confirm the observation that two biological pathways were operating in the para-substituted aniline degradation.

Work on the effect of sorption on the hydrolysis of chlorostilbene oxide (CSO) in different systems is completed and a manuscript is in preparation. Results indicate that sorption to humic materials indeed retard the hydrolysis of CSO, under both acid-catalyzed and neutral conditions.

A manuscript on the method of characterizing sediment redox conditions with indicator dyes is being developed. Oxidation of anaerobic sediment samples during autoclaving was observed in a study using the indicator dyes. Because this phenomenon affects the interpretation of autoclaved control experiments in studies of reductive transformations of pollutants, it has been thoroughly investigated and a brief journal article reporting the results is being prepared.

Dr. Eric Weber and Mr. George Baughman attended an EPA-sponsored Azo Dye and Pigment Regulatory Workshop in Raleigh, NC, on August 15-17, 1988. They presented their latest research findings and participated in discussions to develop a regulatory strategy for azo dyes. In support of this effort, samples from the influent and the effluent of a municipal water treatment plant receiving waste from a North Carolina textile mill were analyzed. Thin layer chromatography indicated the presence of approximately 20 dyes in the influent and 3 dyes in the effluent. The dyes in the effluent are most likely acid or direct dyes. Methodology is currently being developed to separate and isolate the dyes in the effluent sample.

STATUS AND SCHEDULE OF DELIVERABLES:

8051 INTERNAL REPORT ON THE FATE OF ORGANIC POLLUTANTS IN THE SUBSURFACE ENVIRONMENT
DUE: 05/31/88 REVISED: 01/01/00 COMPLETED: 05/31/88

CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: D109 HAZARDOUS WASTE
ISSUE: C WASTE CHARACTERIZATION
PPA (L): 96 Waste Futures and Aquatic Impacts

PPA (S): 96 HW Aquatic Impacts
RC: K ERL ATHNS
PROJECT: 30 Assessment Methods for HW Characteristics and Constituents
PROJ OFFICER: Thomas Barnwell PHONE: 8-250-3175

***** PLANNED START: 01/31/88 PLANNED END: 09/30/95 *****

PROJECT DESCRIPTION:

NO DESCRIPTION AVAILABLE

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The SARAH2 computer code has been tested, and the full-screen editor is nearly complete. The model was presented at CEAM workshops in July and August. Final implementation of the monte carlo shell for SARAH2 is on hold pending completion of testing of algorithms and final development of the new user interface.

Work on a feasibility study on integrating habitat evaluation procedures in SARAH and a draft flooding scenario feasibility study continues.

A screening tool has been developed for estimating effects in streams of oily wastes migrating from Subtitle D disposal facilities. The OWL model documentation (8099A) provides instruction for forward or backward calculation of oily waste concentrations.

The habitat suitability index (HSI) feasibility study, including several examples of using SARAH2 inputs and outputs with HSI models, is under development.

Proposed flooding regulations for solid waste management units were received from OSW and are being reviewed to evaluate future modeling needs.

STATUS AND SCHEDULE OF DELIVERABLES:

2088 INTERNAL REPORT ON PREDICTING AQUATIC HABITAT IMPACTS FROM OILY WASTES
DUE: 03/31/88 REVISED: 01/01/00 COMPLETED: 03/31/88

CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

STATUS AND SCHEDULE OF DELIVERABLES:

8089 INTERNAL REPORT ON MODEL TO PREDICT IMPACT FROM OILY WASTES
DUE: 07/31/88 REVISED: 01/01/00 COMPLETED: 07/31/88

CLIENT OFFICE: OSW

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: D109 HAZARDOUS WASTE
ISSUE: D DIOXIN
PPA (L): 54 MOVEMENT & PERSISTENCE OF DIOXINS IN SOILS & GROUND WATER

PPA (S): 54 DIOXIN TRANSPORT
RC: K ERL ATHNS
PROJECT: 35 Photodegradation of Dioxin in Soils
PROJ OFFICER: Richard G. Zepp PHONE: FIS-250-3428

***** PLANNED START: 10/01/85 PLANNED END: 12/31/99 *****

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 and related compounds 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 and related compounds 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 at the University of Nevada-Reno for the previous three months has revolved around three subprojects:

1. Completion of data collection for a journal article on dioxin photolysis on soils. High-resolution gc-ms data supported conclusions from previous laboratory irradiations of octachlorodibenzodioxin (OCDD) on soils, indicating that tetrachlorodibenzodioxin (TCDD) is produced, albeit at low conversion yields, from OCDD. The levels produced by sunlight irradiations were somewhat lower than those from the indoor irradiations.

2. Effect of weathering on photolysis of organic compounds on soils. Two soils with organic content of 1% organic carbon and 6% organic carbon were exposed to sunlight for a 2-week period. Three compounds were applied to the preexposed soils and soils that had not been exposed to sunlight. These samples then were exposed to sunlight over a 15-day period. No significant difference

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CLIENT OFFICE: OSW

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ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

in degradation rate of the chemicals was apparent between the preexposed and unexposed soils.

3. Effect of added organic on the photolysis of 2,3,7,8-TCDD on soils. TCDD was irradiated on soils containing 0%, 1% and 5% hexadecane. The depth of photolysis was observed to increase substantially for the higher hexadecane levels, suggesting that movement of the TCDD is occurring in the hexadecane film.

Experiments are underway now to determine whether vapor phase movement of organics significantly affects photolysis. The photolysis rates of a series of phenyl ketones with chain length varying from 3 carbons to 18 carbons will be measured on soils to determine whether there is an increase in photolysis rate of the lower molecular weight compounds compared to the higher molecular weight compounds.

STATUS AND SCHEDULE OF DELIVERABLES:

7355 REPORT ON PHOTODEGRADATION EVALUATION OF DIOXIN (2,3,7,8-TCDD) IN SOILS
DUE: 06/30/88 REVISED: 07/31/89 COMPLETED: 01/01/00

CLIENT OFFICE: OPP

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: E104 PESTICIDES
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
PROJ OFFICER: David S. Brown PHONE: FIS-250-3310

***** PLANNED START: 04/01/81 PLANNED END: 03/31/89 *****

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, other agencies to generate requisite data bases to test either complete model 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:

The sampling scheme for the Dougherty Plain site in 1988 was reduced to measuring the ambient environmental parameters and analyzing samples for the bromide tracer in soil and in ground waters.

All sample analyses from the 1987 season have been completed for aldicarb, aldicarb sulfoxide, aldicarb sulfone, and metolachlor levels in soil, water and plants. This represents 1700 samples and a total of 6800 individual pesticide determinations. Also, 1250 samples from the 1987 season have been analyzed for bromide.

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The report "Validation Status of Pesticide Leaching and Groundwater Transport Model" was provided to OPP. One of the key points of the report was the development of a model performance index as a quantitative measure of the predictive capability of a model. The methodology addresses the question of whether model predictions are within a given factor of the true concentration values. It appears that this index will be useful in summarizing model capability and for comparing relative performance of one model versus another.

Results of preliminary testing of PRZM indicate that the model was not able to simulate a perfect fit between the observed and predicted residue concentration profiles for aldicarb, although in several instances the predictions were within confidence bounds. For metolachlor, the model performed relatively much better.

PRZM was found to be sensitive to both degradation rate coefficients and to heavy rainfall events. These observations have implications in regard to analysis of model components (i.e., hydrology, degradation rate) and also with regard to estimation of model parameters and to calibration techniques.

In regard to analysis of pesticide concentrations in soil profiles, there were instances in which the capability index indicated that model predictions differed from true values by a factor of 2 or more, but in most cases PRZM appeared to be capable of predicting with a factor of 2. These observations were consistent over four crop/pesticide application years. The large index values usually were associated with very small observed concentrations. Pesticide movement to deep levels (approaching the water table) was not observed nor was it predicted by PRZM for either aldicarb or metolachlor. The limited movement did not permit an investigation of the deep-zone predictive capabilities of PRZM, although the fact that PRZM did not predict deep movement is consistent with the data.

STATUS AND SCHEDULE OF DELIVERABLES:

- # 7661 FINAL DOUGHERTY PLAIN REPORT INCLUDING PESTICIDE GROUND WATER THREAT ASSESSMENT METHOD
DUE: 09/30/89 REVISED: 01/01/90 COMPLETED: 01/01/90
- # 7664 Project Report on Soils Data Based for RUSTIC Model (Linked PRZM-Groundwater Model)
DUE: 06/30/89 REVISED: 01/01/90 COMPLETED: 01/01/90
- # 8053 INTERNAL REPORT (RESEARCH BRIEF) ON VALIDATION STATUS OF PESTICIDE LEACHING AND GROUND WATER TRANSPORT MODULES
DUE: 08/31/88 REVISED: 01/01/90 COMPLETED: 08/31/88

CLIENT OFFICE: OPP

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: E104 PESTICIDES
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: 14 Pesticide Process Characterization
PROJ OFFICER: Arthur W. Garrison PHONE: FTS-250-3145

***** PLANNED START: 10/01/87 PLANNED END: 12/31/99 *****

PROJECT DESCRIPTION:

GOAL: Characterize key environmental processes that lead to transformation or transport of pesticides in soil, sediment, water and related environments; apply this information to improve predictive techniques for environmental exposure.

RATIONALE: Transformation processes such as redox reactions in anoxic environments (some sediments, subsurface zones), photolysis on soil and plant surfaces and in the vapor state above application areas, and sorption, especially of irrigable pesticides, are not characterized to the extent necessary to account for pesticides loss to the environment. Degradation products are not identified for many processes.

APPROACH: Laboratory studies using natural waters, soils, sediments, and reference materials will be conducted to test proposed equations for pesticide transformation kinetics and sorption equilibria. These studies will provide rate and equilibrium constants required for exposure predictive models. Compounds and reaction conditions will be selected to permit generalizations about changes in molecular structure and environmental conditions. Initially, photochemical transformations on soil surfaces and sorption of water soluble (irrigable) pesticides to soils and sediments will be emphasized.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Results of partitioning of 10 ionizable (anionic) organic compounds between water and octanol as a function of aqueous phase inorganic ion concentration and composition (LiCl, KCl, NaCl, CaCl₂, and MgCl₂) and pH are discussed in a manuscript currently in preparation. The relevance of this work to adsorption behavior (and hence, the ultimate fate and toxicity) of ionizable organic pollutants in the environment is addressed.

Laboratory work investigating sediment-organic anion interactions continues. Partition coefficients have now been measured for two anionic

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FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
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ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Organic compounds (DNOC and silvex) in 12 well-characterized sediments. Although partitioning appears to be strongly influenced by hydrophobic interactions (as expressed by fraction of organic carbon), other system characteristics such as pH and conductivity (a measure of aqueous phase ionic strength) also may influence partitioning.

Preliminary data indicate that the half life of the herbicide basalin in anaerobic sediments is very short. Identification of the degradation product is now in progress. Laboratory work on the fate of phorate sulfoxide in anaerobic sediments is largely complete; a manuscript describing the results is in preparation.

STATUS AND SCHEDULE OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT

CLIENT OFFICE: OPP

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ERL ATHNS: JULY - SEPTEMBER 1988

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CODE  TITLE
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BSA: E104 PESTICIDES
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
PROJ OFFICER: David S. Brown      PHONE: FIS-250-3310
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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 model development activities for QTS and OW are envisioned and required, e.g. PPM assessments.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Activities this quarter concentrated on model development. The linked groundwater-leaching model, designated as RUSTIC, is undergoing comprehensive review and testing (beta tests and sensitivity tests). The overall model includes an enhanced PRZM, a one-dimensional unsaturated zone module, and a two-dimensional saturated zone module. Presently, the model runs on the Agency's DEC-VAX but is too large for operation on personal computers.

Other activities this quarter concentrated on assisting OPP in changing their runoff modeling from the SWRRB-based approach (an OPP model) to a similar approach based on PRZM. This conversion should enable more uniform exposure assessments by analyzing runoff, leaching, and ultimately terrestrial problems

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ERL ATHNS: JULY - SEPTEMBER 1988

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:
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with the same basic tool.

STATUS AND SCHEDULE OF DELIVERABLES:
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# 7709 Users Manual for Exposure Assessment Model of Pesticide Contamination of
Ground Water
DUE: 06/30/88 REVISED: 01/01/00 COMPLETED: 06/30/88
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CLIENT OFFICE: OPP

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: E104 PESTICIDES
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
PROJ OFFICER: David S. Brown PHONE: FIS-250-3310

***** PLANNED START: 10/01/85 PLANNED END: 12/31/99 *****

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 probabilities and uncertainties associated with real world problems. Close coordination will be required with CERL, RSKERI, ASRL-RTP and the aquatic fate research at AERL.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A user's manual (7977A) has been developed for a computerized methodology to assess potential toxic chemical exposures to terrestrial wildlife. The Terrestrial Ecosystem Exposure Assessment Model (TEEAM) is a major product of the Ecological Risk Assessment Research Program.

While on IPA assignment at Oregon State University (OSU), Dr. David S. Brown investigated several possibilities for further development and testing of TEEAM with Dr. Bill Williams and other ERL-Corvallis staff and several members of the Critical Ecosystem Project research group in the Oregon State Botany and Plant Pathology Department. Dr. Elaine Ingham (OSU) is developing detailed food

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ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

chain relationships for the highest ranked critical ecosystem (dryland wheat). The information is expected to be useful in planning future field tests and compiling species-specific input data for TEEAM's Markov transition probability matrix.

A series of sensitivity tests on major variables in TEEAM was conducted. The total variability of model outputs is associated with a small number of key input variables. It appears that pesticide application rate is the most important variable.

STATUS AND SCHEDULE OF DELIVERABLES:

7977 USERS MANUAL FOR TERRESTRIAL ECOSYSTEM EXPOSURE ASSESSMENT MODEL (TEEAM)
DUE: 08/30/88 REVISED: 01/01/00 COMPLETED: 08/30/88

CLIENT OFFICE: OTS

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ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: L104 TOXICS
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION
PPA (L): 09 DEVELOPMENT OF VALIDATED EXPOSURE ASSESSMENT METHODOLOGIES

PPA (S): 09 EXPOSURE ASSESSMENT
RC: K ERL ATHNS
PROJECT: 12 Development of EcoRisk Exposure Models
PRGJ OFFICER: Craig Barber PHONE: FTS-250-3147

PLANNED START: 10/01/87 PLANNED END: 12/31/99

PROJECT DESCRIPTION:

GOAL: To provide modeling approaches for evaluating exchanges of toxic chemicals between aquatic organisms and their environment.
RATIONALE: The evaluation and prediction of risk from toxicants must be based on sound methods for assessing the uptake, distribution, and effects in target organisms. Testing all chemicals would be impossible and models must be developed which can use readily available chemical parameters to make predictions.
APPROACH: Exchange models will be developed to provide estimates of body burdens of candidate chemicals. Models will be based on thermodynamic principles and morphometric characteristics of organisms as well as taking into consideration route of exposure (water, food, or benthic sediments). Assessments can then take into account multiple sources of contaminants and also be extended to include ecological significance or effects. Physiological response depends on the chemical concentration in the organisms rather than that in the environment and the exchange models will be linked to toxicokinetic models to predict effects. Laboratory experiments will be conducted to test underlying hypotheses, and other factors involved will be identified.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

An article (7900A) describing the passive accumulation in fish of organic chemicals in environmental waters and in contaminated prey was submitted for publication in the Canadian Journal of Fisheries and Aquatic Sciences. The work represents a continuing enhancement of the Food and Gill Exchange of Toxic Substances (FGETS) model.

FGETS was presented at two EPA Center for Exposure Assessment Modeling workshops that were held this quarter in Washington DC, and Boulder, CO. It was well received at both presentations. As a result of discussions with workshop participants, some of FGETS user interface was modified to facilitate multiple

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

simulations. FGETS also was presented at the Food Chain Workshop held at ERL-Athens in conjunction with the CEAM's involvement with the Green Bay PCB project.

A database working group composed of scientists from ERL-Athens, Computer Sciences Corporation, and the University of Georgia continued biweekly meetings this quarter in a project to develop software for a Geographic Information System for exposure assessment. This software will interface EXAMS and FGETS with a GIS that will identify species at risk.

In August, Dr. Barber attended a Human Health (Cancer) Risk Assessment Workshop sponsored by EPA Region IV and discussed the FGETS model. As a result, Mr. Ron Landy, a toxicologist in Region IV who attended the meeting, became very interested in the possibility of applying FGETS in some of his work. Assistance in using FGETS will be provided.

STATUS AND SCHEDULE OF DELIVERABLES:

7900 JOURNAL ARTICLE ON A MODEL DESCRIBING THE UPTAKE OF NONPOLAR XENOBIOTICS FROM CONTAMINATED FOOD
DUE: 07/31/88 REVISED: 01/01/00 COMPLETED: 07/31/88

CLIENT OFFICE: OTS

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OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE
BSA: L104 TOXICS
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION
PPA (L): 03 DEVELOPMENT OF VALIDATED EXPOSURE ASSESSMENT METHODOLOGIES
PPA (S): 03 EXPOSURE ASSESSMENT
RC: K ERL ATHNS
PROJECT: 27 Development of Validated Exposure Assessment Methodologies
PROJ OFFICER: Robert B. Ambrose PHONE: FIS-250-3546

***** PLANNED START: 10/01/79 PLANNED END: 12/31/99 *****

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: OTS wants to upgrade its metals and organics multimedia modeling capability for PPM 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 (particularly intermedia) and transformation kinetics of pollutants will be incorporated into multimedia models to produce more reliable exposure assessment packages for organics of interest under TSCA and RCRA.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The University of Florida delivered a standard Fortran-77 computer code of the 3-D estuary and lake hydrodynamic model to EPA. The code has been well tested and documented. A new feature is an option to do simulation on a user-specified non-uniform grid, which does not require the generation of the so-called "stretched" grid through the solution of non-linear equations. This feature will be implemented for the Green Bay application. In this regard, the University of Florida will maintain a close working relationship to assist EPA's model application throughout the study period. During the coming quarter, the University of Florida will begin implementation of the sediment dispersion model.

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The Lake Okeechobee field work designed to generate sediment movement data for modeling is completely ready after a recent delay due to Hurricane Gilbert. The University of Florida's field crew is going to spend a week at the lake installing platforms and instruments. Intensive data at 2Hz frequency will be collected. The month of October will be spent conducting synoptic surveys to collect data of suspended sediment concentration and phosphorus.

STATUS AND SCHEDULE OF DELIVERABLES:

8047 FINAL REPORT ON MONTE CARLO VERSION OF MINTEQ
DUE: 08/31/89 REVISED: 01/01/00 COMPLETED: 01/01/00

CLIENT OFFICE: OTS

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ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: L104 TOXICS
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: 09 Chemical Process Characterization for Toxics
PROJ OFFICER: Richard G. Zepp PHONE: FTS-250-3428

PLANNED START: 10/01/79 PLANNED END: 09/30/99

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 and equilibria of transformation processes. The laboratory studies will provide rates and equilibrium constants to fill the equations. Compounds and reaction conditions will be selected to permit generalizations about changes in molecular structure and environmental composition. Photochemical studies will emphasize role of naturally occurring inorganic species; redox reactions of abiotic systems, relative to biotic systems, will be studied.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Studies continue on the hydrolysis of Disperse Blue 79 in activated sludge. The rates of hydrolysis of purified Disperse Blue 79 and the commercial dyestuff (26% in Disperse Blue 79) were compared. Purified Disperse Blue 79 is hydrolyzed with a half-life of 30 minutes; however, no hydrolysis was observed for the dyestuff over a 5-day period. These results suggest that the dispersing agents present in the dyestuff are complexing Disperse Blue 79 and preventing it from making contact with the surface of the sludge where hydrolysis takes place. These results may explain the observation that as much as 20% of Disperse Blue 79 dyestuff passes through a model waste water treatment plant (Glen Shaul, WERI, EPA, Cincinnati, Ohio).

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Work also has progressed on the analysis of samples taken from the influent and the effluent of a municipal treatment plant receiving waste from a textile mill in North Carolina, N.C. area. Thin layer chromatography indicates the presence of approximately 20 dyes in the influent and 3 dyes in the effluent. The dyes in the effluent are most likely acid or direct dyes. Methodology is currently being developed to separate and isolate the dyes in the effluent sample.

Dr. Eric of ERL-Athens Weber attended an EPA-sponsored Azo Dye and Pigment Regulatory Workshop in Raleigh, NC, on August 15-17, 1988. Weber presented his latest research findings and participated in discussions to develop a regulatory strategy for azo dyes.

Dr. Weber and Mr. George Baughman organized and co-chaired a symposium at the National Meeting of the American Chemical Society in Los Angeles, CA, on September 25-30, 1988 entitled "Environmental Chemistry of Dyes." Weber presented a paper on the reduction of Disperse Blue 79 in anaerobic sediments.

Studies on the role of trace metals in photochemical redox processes continue with work involving iron, copper and manganese. Two types of studies are being pursued involving iron. One is concerned with the effects of various environmental variables on the rate of oxidation and/or reduction of iron in aqueous solution. The reduction of iron (III) in the presence of fulvic acid was faster at higher pH, and the rate increased with irradiation at 436 nm. The second group of iron studies involves the degradation of several organic substrates in the presence of iron, hydrogen peroxide and octanol with sunlight. The substrates examined were, in order of decreasing reactivity, p-nitrophenol, p-cresol, nitrobenzene, and atrazine. Other substrates will be tested using the same system.

Studies of the reactions of manganese oxides with phenols are continuing. Previous work indicated that the oxidation of several phenols by MnO₂ was enhanced by sunlight, and that the reaction rates increased with decreasing pH. This quarter, the dark-state reactions of p-chlorophenol with MnO₂ at pH 4.2 were examined; the disappearance of p-chlorophenol was faster with Mn(IV) than with Mn(III). These experiments will be repeated using light.

STATUS AND SCHEDULE OF DELIVERABLES:

7902 REPORT (RESEARCH BRIEF) ON FATE OF TEXTILE DYES IN THE AQUATIC ENVIRONMENT
DUE: 03/31/88 REVISED: 01/01/00 COMPLETED: 03/31/88

CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: L104 TOXICS
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
PROJ OFFICER: William C. Steen PHONE: FTS-250-3776

***** PLANNED START: 10/01/85 PLANNED END: 12/31/99 *****

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. 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 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:

Second-order microbial transformation rate constants were determined for the two remaining para-substituted acetanilides (p-cyano and p-bromo acetanilide) previously selected from the list chosen for the 2% set-aside project to establish spectroscopic-based property-reactivity correlations. The table below lists the chemicals studied to date and their calculated second-order microbial degradation rate constants.

SUBSTITUTED ACETANILIDE (Para Position)	MEAN SECOND-ORDER RATE CONSTANT (L/Org./Hr.)
Chloro	1.11 E-10(4)
Methyl	5.00 E-11(4)
Bromo	3.85 E-11(4)
Nitro	2.20 E-12(4)
Methoxy	8.51 E-13(4)

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FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Cyano 1.45 E-13(4)

(4) = No. of determinations

The last of the selected acetanilides is being investigated using Hickory Hill Pond water and will complete this series of chemicals.

Measurements with the Standard Reference chemical, propanil, are continuing as well as an additional substituted amide (nicrosamide).

During the quarter as part of the US/USSR Project: 02.03-31 "Fate and Transport of Pesticides in the Environment" Dr. William C. Steen spent July 4-31 working within the Institute of Soil Science and Photosynthesis in Puschino USSR with Dr. Nadia Anan'eva. The work involved investigating the microbial transformation of metalaxyl, a fungicide, in both aqueous and sediment/water systems. The objectives of these investigations were to measure the second-order microbial rate constant and to evaluate an indirect measure of bacterial density using respirometric measurements. The results of this work, being concluded within the Institute in Puschino, will be reported during the coming year.

STATUS AND SCHEDULE OF DELIVERABLES:

7282 REPORT ON MICROBIAL TRANSFORMATION RATE CONSTANTS
FOR SUSPENDED POPULATIONS
DUE: 03/30/87 REVISED: 12/31/87 COMPLETED: 12/31/87

CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE
BSA: L104 TOXICS
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: 05 Chemical Transformation and Equilibrium Constants
PROJ OFFICER: Heinz Kollig PHONE: FIS-250-3770

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

PROJECT DESCRIPTION:

GOAL: Establish and maintain data bases in which data are of known reliability for use in risk assessments, either as "analogs" or as inputs to exposure algorithms, and in expert systems for estimating physical, chemical and microbial constants. Communicate data to the user community.
RATIONALE: Scientifically valid and accurate transformation rate and equilibrium constants are required as inputs to mathematical models and other decision tools to assess risk associated with toxic and other hazardous chemicals.
APPROACH: A data base management system will be established that can meet user needs. Data will be acquired from the following sources: (1) The literature, (2) Manufacturers' data submissions to EPA (3) Computations made by technicians and (4) Inhouse laboratory measurements. All data will be screened for reliability by applying previously established criteria.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The manuscript "A Fate Constant Data Program," by Heinz P. Kollig, was submitted for publication in Environmental Monitoring and Assessment.

The Coordinated List of Chemicals (CLC) database was distributed to all ORD laboratories and to EPA offices expressing interest, including the Regional Scientist Coordinator (Dr. Michael Moore). Information retrievable from the database will tell who is studying what chemical in ORD. CLC stores 1751 chemicals and was distributed on diskettes for use on personal computers. Developed originally to help the ERL-Athens assure relevancy of its chemical property information, the database has significant potential in coordinating research and providing information to regions and program offices.

In order to apply property-reactivity relationships between infrared spectra and chemical or microbial transformation rates for the purpose of

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CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

predicting rates of new chemicals, it is necessary to define what constitutes a "chemical class." Once defined, the infrared spectrum of a compound whose transformation rate is unknown can be compared to that of the base compound representing the appropriate chemical class. To define chemical classes, a four-person committee examined the feasibility of classifying 300 to 500 chemicals constituting two lists of EPA-regulated compounds. (Classifying a larger population of chemicals initially is impractical.) Abiotic hydrolysis was the transformation process considered, and the reactive moiety was chosen as the basis for classification. The committee has determined, at this point, that the classification process is feasible and will continue its deliberations.

Mr. Kollig was invited by the National Agricultural Chemical Association to participate in a steering committee meeting to discuss the development of a pesticide fate database with emphasis on data quality for the Agricultural Research Service, USDA. Representatives from different divisions of USDA, EPA's OPP, industry, and academia participated. The work we are doing to evaluate data quality drew strong interest from the committee.

continued...

DATE: 11/18/88 Program Management System PAGE: 54
PMS-062 Office of Research and Development Information Systems

CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

DATE: 11/18/88 Program Management System PAGE: 55
PMS-062 Office of Research and Development Information Systems

CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

11B101B23P.12B101B23P.13B101B23P.14B101B23Q.20B101B26N.29B101B26N.33B101B

STATUS AND SCHEDULE OF DELIVERABLES:

- # 7710 Interim Protocol for Measurement of Hydrolysis Rate Constants
DUE: 03/31/88 REVISED: 01/01/00 COMPLETED: 03/31/88
- # 7905 Report on problems associated with published environmental fate constants
DUE: 03/31/89 REVISED: 01/01/00 COMPLETED: 01/01/00

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CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: L104 TOXICS
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
PROJ OFFICER: Harvey W. Holm PHONE: FIS-250-3103

PLANNED START: 10/01/79 PLANNED END: 12/31/99

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 hazard 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:

Laboratory experiments are continuing to test the hypothesis of a threshold critical aqueous blood concentration of a test chemical (1,2,3,4-tetrachlorobenzene-TCB) at which death of an organism occurs. Additional channel catfish have been exposed to lethal concentrations of TCB and sampled at various times to determine whether there is a defined endpoint before death or if death is the only proper endpoint. The data are still inconclusive at this point.

Another species of fish, bluegill sunfish (*Lepomis macrochirus*), is now being tested in lethal concentrations of TCB (1.9 to 3.1 mg/l). The same problem of nonuniform endpoint has been observed with this species. The fish turn over within 1 to 2 hours and then slowly decrease activity until absolute cessation of ventilation up to 50 hours later. If a specimen is removed from the test tank after 48 hours while still ventilating even very slowly, and put

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CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

into clean water, it recovers. Results are inconsistent for living, dying and dead fish. It appears that the test chemical, a narcotic, is influencing metabolism and the process of dying in these fish. A review of this work was presented at a workshop "Food Chain Modeling and Experimental Verification" at ERL-Athens in September.

STATUS AND SCHEDULE OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT

CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: L104 TOXICS
ISSUE: G STRUCTURE ACTIVITY RELATIONSHIPS
PPA (L): 20 STRUCTURE-ACTIVITY RELATIONSHIPS AND ESTIMATION TECHNIQUES

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

***** PLANNED START: 10/01/80 PLANNED END: 12/31/99 *****

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/equilibrium constants to molecular structure will be developed for direct photolytic and hydrolytic transformation and for acidity constants (pKa). 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:

Two refinements are being made in SPARC, the ERL-Athens expert system for predicting chemical reactivity parameters:

1) Since the quality of computational output necessarily reflects the quality of calibration of parameters in any successful quantitative chemical model, a "self-training" algorithm called TRAIN has been developed for SPARC. The program takes a set of target model parameters (initial values plus any appropriate boundary values) together with a set of designated data and provides an optimized set of model parameters. TRAIN cycles through a Jacobian optimization procedure, then sets up and executes the specifics of optimization as requested by the user.

2) A performance validity (PV) program module is being written to assure that all computational elements in SPARC are working at optimum by being sub-

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CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

jected to a variety of compounds (about 100) that represent different types of molecular reactivity. The nature of these representative compounds is such that all types of computation in the system are checked for evidence of any "rippling" effect that might remain unnoticed in the system. The purpose of PV is to sustain the validity of program code and performance as the total system (SPARC) is being developed. This will enhance confidence in the system as algorithms for other chemical reactivity parameters (hydrolysis, Kow, redox, etc.) are being developed.

Coding and input of compound pKa's into the data base is continuing. To date, 3067 compounds have been entered.

STATUS AND SCHEDULE OF DELIVERABLES:

7917 REPORT ON TECHNIQUES FOR USING CHEMICAL PROPERTIES TO ESTIMATE
PHOTOCHEMICAL RATE CONSTANTS
DUE: 06/30/88 REVISED: 01/01/00 COMPLETED: 04/30/88

8048 INTERNAL REPORT (RESEARCH BRIEF) ON EXPERT SYSTEM TO ESTIMATE REACTIVITY
PARAMETERS FOR ORGANIC POLLUTANT TRANSFORMATION
DUE: 08/31/88 REVISED: 01/01/00 COMPLETED: 04/30/88

CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: L104 TOXICS
ISSUE: 9 STRUCTURE ACTIVITY RELATIONSHIPS
PPA (L): 20 STRUCTURE-ACTIVITY RELATIONSHIPS AND ESTIMATION TECHNIQUES
PPA (S): 20 SAR/EST TECHNIQUES
RC: K ERL ATHNS
PROJECT: 15 PRC Relationships and Other Estimation Techniques
PROJ OFFICER: Harvey W. Holm PHONE: FTS-250-3103

***** PLANNED START: 05/01/83 PLANNED END: 09/30/99 *****

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:

(1) Theoretical Analysis of Monod Kinetics. The Monod equation was integrated to obtain the theoretical kinetics of cell number increase and simultaneous substrate disappearance during substrate (e.g., xenobiotic) limited cell growth. Computer graphics of the theoretical kinetics were generated. At substrate concentrations below the half-maximal constant ($S_0 \ll K_s$), the $t_{1/2}$ for the first-order degradation of substrate is identical to the doubling of cell number (G). At $S_0 > K_s$, G is not identical to $t_{1/2}$. The computer graphics show that as the ratio S_0/K_s decreases, G and $t_{1/2}$ increase, as predicted by the Monod equation. In future studies, the measured kinetics of xenobiotic degradation in river water will be curve-fit to the theoretical Monod kinetics. If the kinetics of both xenobiotic degradation and cell number increase are found to fit the Monod equation, then the xenobiotic is converted into biochemical energy and degradation is likely to involve complete oxidation of the carbon portion to carbon dioxide. Potentially toxic side products are

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CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

not likely to accumulate.
An automated spectrophotometric assay was adapted to measure the kinetics of cell number increase. The extinction coefficient of cells in river water was 1.1×10^9 Abs/(cells/ml). The spectrophotometric assay provides a measure of C_0 , the number of cells at zero time, by back extrapolation of the kinetics. The spectrophotometric assay will supplement the known assays for cell number -- cell plate (CFU) counts and acridine orange staining followed by microscopic counting. In some cases the spectrophotometric assay is easier and generates more complete kinetic curves.

(2) Analytical Characterization of River Water. Standard tests are being implemented to characterize river water each time a sample is taken. To date it is concluded that one sample of river water has the following properties/composition: $T = 25.8^\circ\text{C}$; pH 6.9; 0.6 mM unknown buffer, pKa 6.4; estimated 3.6 mg/L humic + fulvic acids (based on UV-VIS spectra of river water and commercially purified humic/fulvic acids); 96% polar compounds (by LC/UV).

(3) Characterization of Cell Strains in River Water. Cells in river water are being analyzed for cell number, strain identity, and strain frequency. The CFU/plate count is dependent on the time of incubation of the plates up to 4 days. This variable was eliminated by counting plates after 6 days. Storage of river water above 0°C yielded a 4-fold (4°C) to 8-fold (25°C) increase in CFU/ml after two days after which cell number was stable for 40 days, whereas storage at 0°C resulted in a 40-fold loss of cells. Strain variability, analyzed by visual inspection of agar plates, appeared constant for river water stored at 25°C and 0°C for 42 days (> 8 strains), but decreased upon storage at 4°C . Thus, surprisingly, the best conditions to maintain river water at or near its original state appears to be 25°C (room temperature) based on these preliminary findings.

STATUS AND SCHEDULE OF DELIVERABLES:

7916 Report: Current use of structure activity relationships for predicting biotransformation of chemicals
DUE: 08/31/88 REVISED: 08/31/89 COMPLETED: 01/01/00

CLIENT OFFICE: AA OPTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: L104 TOXICS
ISSUE: I ECOLOGY: ECTOXICITY 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
PROJ OFFICER: Ray R. Lassiter PHONE: FIS-250-3208

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

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:

Studies on the uptake of neutral, hydrophobic xenobiotics and on the relationship of the process to uptake of oxygen are progressing in an EPA cooperative agreement with Montana State University (MSU) and the University of British Columbia (UBC). After completing preliminary exposure studies of 1,1,2-trichloroethane (TCE) in the respirometer at UBC, tissue samples were taken to MSU for analysis. Analyses of TCE proved difficult, costly, and imprecise, and studies were halted in favor of conducting exposures using a higher log P chemical, 1,2,4,5-tetrachlorobenzene (TCB).

Preliminary studies indicate few problems with the TCB analyses, but the TCB dissipates in the respirometer (half-life of about 1 hr). Different swimming speeds were used for rainbow trout (RBT) exposed to TCB, and oxygen utilization was monitored. Individual fish were exposed for 1 to 12 hours and then sacri-

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CLIENT OFFICE: AA OPTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

ficed, dissected, frozen and taken to MSU for analysis. As expected, adipose tissue had the highest concentration of TCB, and levels increased with time. Concentrations in other tissues were more variable and further studies to determine the three best tissues to monitor are underway. A review of this work was presented at a workshop on "Food Chain Modeling and Experimental Verification" at ERL-Athens in September. More definitive studies on uptake are proceeding and studies in the respirometer on sublethal effects as measured by stamina under a swimming stress will begin next quarter.

The cooperative agreement with The University of Georgia is proceeding on schedule. Data structures for databases to support aquatic ecosystem models and dBASE3 files containing FGETS physiological parameters for various fish species are being evaluated by the EcoRisk group.

Two manuscripts, "Survival of the Fattest: A Theory for Assessing Acute Effects of Hydrophobic Chemicals on Populations" and "Determination of Effects of Lipophilic Toxicants on the Dynamics of Daphnia Populations," were submitted for publication in Environmental Toxicology and Chemistry. Development of the physiologically structured population model for fish, which is analogous to the Daphnia model described in the aforementioned manuscripts, continued.

A qualitative sensitivity analysis of the TOX effects model was conducted this quarter. Although we have previously hypothesized that much of the difference in species susceptibilities could be explained largely by species-to-species variations in lipid content, results of these analyses suggest that differences in gill morphometry also may be the basis for as much if not more of species-to-species variation in acute toxicity tests. Development of a user friendly PC interface for TOX was started. This interface will be completed early next quarter.

To help facilitate user input to TOX, FGETS, and other EcoRisk models, a units conversion program for the PC has been developed. The interactive version of this program is now complete. Next quarter, a driver program that will allow its use with specific models will be developed.

In an article in preparation, experimental observations on the bioconcentration of two chlorobenzenes in three plant species are compared to model simulations that predict chemical exchange based on fugacity gradients, plant morphology, and plant proximate composition. Partitioning experiments using three different extracts of Hydrilla verticillata were conducted also to determine the magnitude of chemical partitioning into nonlipid, structural plant parts.

OPP has requested assistance in generation of appropriate databases for

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CLIENT OFFICE: AA OPTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

evaluation of pesticide impacts in small watersheds. A proposed physical configuration was submitted for evaluation. Also requested was a set of small modifications to EXAMS to automate some of the more mechanical estimation procedures for dealing with missing data. A modest modernization program, designed to incorporate recent advances in microbial and chemical kinetics will be undertaken early in October to keep EXAMS at the state-of-the-art for continued use by OPTS programs. Activities under this project also include continued oversight of the biota database, and continued study of the potential role of Geographic Information System technology for furtherance of OPTS regulatory program needs.

STATUS AND SCHEDULE OF DELIVERABLES:

- # 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: 01/01/00
- # 7512 DOCUMENTATION REPORT ON SPECIFICATIONS FOR INPUT PARAMETERS AND COMPUTER CODE FOR AQUATIC ECOSYSTEM MODELS
DUE: 08/31/88 REVISED: 08/31/90 COMPLETED: 01/01/00
- # 7513 COMPUTER CODE FOR FIRST OPERATIONAL VERSION OF AN ECOLOGICAL EFFECTS MODEL FOR AQUATIC ECOSYSTEMS
DUE: 08/31/90 REVISED: 08/31/92 COMPLETED: 01/01/00
- # 7514 REPORT ON STATISTICAL ANALYSIS OF TESTS OF ECOSYSTEM MODEL
DUE: 08/31/91 REVISED: 08/31/93 COMPLETED: 01/01/00

CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: L104 TOXICS
ISSUE: I ECOLOGY: ECTOXICITY 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
PROJ 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: Existing software will be reviewed including GEMS, ANNIE, and the IIASA-IRIMS system. Relational data bases will be assembled and prototype risk assessment modeling systems will be developed 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:

The PC-GEMS documentation has been transmitted to OTS as an internal report.

Work on the prototype decision support system this quarter has concentrated on integrating WASP/FGETS, SARAH, and PRZH into the system. The WASP/FGETS module will include three loading scenarios (pulse load, uniform load, time-variable load). Chemical selection will be from the EXAMS chem.dat file. River-reach selection will be from several rivers; fish species selection is from the FGETS data base.

The principal investigator will obtain the new PRZM code (subset of RUSTIC)

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CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

and design a new graphics interface compatible with the GKS graphics standard
used on SUN and DEC VAX/GPX work stations.

STATUS AND SCHEDULE OF DELIVERABLES:

7919 USERS MANUAL FOR SARAH 2
DUE: 05/31/88 REVISED: 01/01/90 COMPLETED: 05/31/88

CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: L104 TOXICS
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
PROJ OFFICER: Lee Mulkey PHONE: FTS-250-3160

PLANNED START: 10/01/79 PLANNED END: 12/31/99

PROJECT DESCRIPTION:

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" exhouse 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, consultation, and assistance to "integrated toxics" projects will also be provided under this project.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The Alaska Department of Environmental Conservation was provided with guidance on precautionary practices for the application of pesticides--veipar and garlon--along railroads.

Mr. Jonathan Naimon, Economic Analysis Staff, Office of Solid Waste, requested an analysis of exposure to wood preserving chemicals in streams near lumber treatment facilities. Two "typical" sites were chosen--one in Georgia and one in Washington. We obtained precipitation, soil, and streamflow data for these two sites. Chemical partitioning data for pentachlorophenol and creosote (benzo(a) pyrene used as surrogate) were estimated. Several simulations of runoff and erosion were performed. Runoff and erosion loads were imported into

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CLIENT OFFICE: OTS

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

a computer spreadsheet and matched with daily USGS stream flow data to produce daily dissolved and particulate stream concentrations. Averages and cumulative distribution functions were produced and plotted. Dissolved concentrations were passed to FGETS to predict bioaccumulation in trout.

Dr. Steve McCutcheon participated in a workshop on "Development of Leach Tests for Contaminate Dredge Material," June 22-24, 1988, at the invitation of the U. S. Army Corps of Engineers.

Mr. Carl Rushchyer, State of California, requested information about arsenic/boron/molybdenum wasteload allocation in alkaline lake-point and non-point sources. We recommended WASP and MINTEQ. He will review manuals and see whether MINTEQ handles arsenic in an alkaline environment and whether boron and molybdenum are in the data base for MINTEQ. Additional assistance will be provided if data indicate that hydrodynamics need to be known or if help is needed with MINTEQ.

At the request of Mr. Peter W. Schaul, Assistant Chief, Hazardous Waste Enforcement Branch, Region III, a draft remedial investigation report on Autco Fibers Superfund site in Front Royal, VA, was reviewed. Dr. Jackson Ellington and Dr. James Martin attended a meeting with responsible parties in Region III. Expert opinion on investigations, degradation processes, and needed work was provided via teleconference and written report.

Mr. Ron Landry, Region IV, requested technical information on runoff of metals. The screening manual was shown to him; PRZM, MINTEQ, other models, and CEAM briefing material were discussed and provided to him. He plans to visit every Friday to learn exposure assessment techniques from us.

Ms. Jackie Burton, Argonne National Laboratory, visited on September 8 to discuss possible applications of MINTEQA2 as a replacement for the EQ3/EQ6 approach they have been using.

Assisted Mr. Jerome L. Pitt, Water Management Division, Region VII, in formulating a MINTEQA2 modeling scenario for estimating dissolved lead in drinking water originating from solder joints. We performed a sample run to get him started.

STATUS AND SCHEDULE OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT

CLIENT OFFICE:

FOURTH QUARTER STATUS REPORT ON FY'88 PROJECT DESCRIPTIONS
OFFICE OF ENVIRONMENTAL PROCESSES AND EFFECTS RESEARCH
ERL ATHNS: JULY - SEPTEMBER 1988

CODE TITLE

BSA: 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

PROJ 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

STATUS AND SCHEDULE OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT

CLIENT OFFICE: OERR

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CODE TITLE

BSA: Y105 SUPERFUND
ISSUE: F PROVIDE TECHNICAL SUPPORT TO ENFORCEMENT, PROGRAM & 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
PROJ OFFICER: Harvey W. Holm PHONE: FIS-250-3103

PLANNED START: 03/30/87 PLANNED END: 12/30/99

PROJECT DESCRIPTION:

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

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The extramural project with PEI and ICF to convene a workshop of scientists to make recommendations for improving the ecological factors of the hazard ranking system (HRS) has been completed. A pre-workshop discussion paper with supporting documentation was produced by the contractors. They also tabulated the recommendations of the scientists at the workshop and combined them with information from their own previous work and work on this project to produce a list of recommendations for use by the Office of Emergency and Remedial Response for revising the HRS. By incorporating as many of the recommendations as practical, the HRS should be able to better discriminate between sites and also be on a firmer scientific and ecological basis. A summary project report is in

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PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

preparation.

A good preliminary selection of tapes, sample extracts, and report packages was made and has been received from the Superfund Sample Management Center and various contract laboratories for the pilot study of Tentatively Identified Compounds (TICs). There were two anticipated problems regarding our ability to examine the tapes: the first, which was considered to be more serious, was that the tapes made on HP GC/MS systems might not be readable by either the VAX or our SuperIncocs; the second, considered less serious, was whether we might have trouble reading data from the most recent Incos system, which is now in use in many contractor laboratories. It now appears that those laboratories having HP systems are willing to prepare the tapes for us in a format that can be read by both the VAX and our laboratory computer; this avoids the first problem. The second problem is both surprising and serious. We are unable to read the Incos 5100 data tapes on our older system. Mr. Myron Stephenson of Region IV also has found that his newest Finnigan GC/MS is unable to read files from the older SuperIncocs systems. He has just received a 9-track magnetic tape unit and is about to evaluate whether he can use this as a means of transferring files. If he is able to do so, he will attempt to translate some of our contractor laboratory tapes for us. The Superfund tapes that can be read have been given a preliminary screening on the VAX. The HIT and reference databases are being modified to reflect the new internal standards, columns, and conditions.

STATUS AND SCHEDULE OF DELIVERABLES:

7966 Report on recommendations for improving the ecological factors of the hazard ranking system
DUE: 02/28/89 REVISED: 01/01/00 COMPLETED: 01/01/00

CLIENT OFFICE: OMPE

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 BSA: Y105 SUPERFUND
 ISSUE: F PROVIDE TECHNICAL SUPPORT TO ENFORCEMENT, PROGRAM & REGIONS
 PPA (L): 22 Enforcement and Other Technical Support/EPE
 PPA (S): 22 Technical Support
 RC: K ERL ATHNS
 PROJECT: 23 Anaerobic Biotreatment Development/SF
 PROJ OFFICER: John E. Rogers PHONE: FIS-250-3592

 PLANNED START: 09/30/87 PLANNED END: 12/31/99

PROJECT DESCRIPTION:

GOAL: Characterize and identify basic biological processes that lead to the anaerobic degradation or detoxification of hazardous wastes in contaminated sites.
 RATIONALE: This research is required to produce a reliable approach to the selection and use of biotreatment processes in the remediation of contaminated hazardous waste sites.
 APPROACH: Pathways and mechanisms for the anaerobic degradation of hazardous organic chemicals will be characterized and identified in environmental samples. Anaerobic consortia capable of growth on these compounds will be enriched from the environment. The key microorganisms in the consortia will be isolated and identified. Key organisms will be added back to the environmental samples to determine whether they enhance degradation of hazardous organic chemicals.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Under a cooperative agreement with Dr. Lily Young at New York Medical Center, we have determined the stoichiometry of the degradation of p-cresol under denitrifying, sulfate reducing, acetogenic and methanogenic conditions. Using specific metabolic inhibitors, we have been investigating the relative importance of different microbial components of the individual enrichment cultures. Results from these studies will be important in determining which organisms are key to the anaerobic bioremediation of hazardous waste sites.

Under the new program "Development of anaerobic biosystems for the treatment of hazardous organic chemicals: degradation of hazardous organic chemicals" we have initiated studies to investigate the degradation of pentachlorophenol (PCP) in anaerobic sediments. Under methanogenic conditions, PCP was degraded within 7 days in sediment adapted to the degradation of 2,4- and 3,4-dichlorophenol. Unacclimated sediments were less active but did completely degrade

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 PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

PCP. Degradation was observed with sediments from the Athens area, the East River in New York City, and in two sediments from the Soviet Union (near Moscow and near the Black Sea).

Initial work has begun on the program "Effect of sorption on the biological remediation of hazardous organic chemicals in soils, sediments, and subsurface materials; enhanced remediation through the use of surfactants and solubilizing agents." The work will describe the influences various surfactants have on the extent to which (toxic) organic chemicals partition between solid phases (e.g., soils, sediments, and aquifer material) and water. Whereas a considerable amount of information is available on solubilization of hydrophobic compounds by micelles, an initial literature search uncovered little on the interactions of surfactants and toxic chemicals in the groundwater environment. The literature, however, does reveal factors of specific surfactants, as well as classes of surfactants (anions, cationic, amphoteric, etc.), that will be important in choosing surfactants for experiments. Initial studies will focus on a dichlorobenzene isomer and on 4,6-dichlorophenol, using sodium dodecyl sulfate in well characterized media.

STATUS AND SCHEDULE OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT

DATE: 11/18/88 Program Management System PAGE: 14
PMS-062 Office of Research and Development Information Systems

CLIENT OFFICE: OERR

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PPA (S): 22 Technical Support
RC: K ERL ATHNS
PROJECT: 29 Center for Exposure Assessment Modeling
PROJ OFFICER: Lee A. Mulkey PHONE: FTS-250-3160

***** PLANNED START: 08/01/87 PLANNED END: 12/30/99

PROJECT DESCRIPTION:

GOAL: To provide regional technical support, expert advice, specialized training, and new methods to conduct exposure assessment modeling for CERCLA sites. For ecological impact need, risk assessment assistance will be provided. Emphasis is on site-specific modeling support and review.
RATIONALE: Exposure assessment modeling technology for human and ecological risk is under development or completed. Application and transfer of such technology has been limited because the requisite highly specialized expertise has not been available or accessible to the Regions and their consultants. Providing a dedicated, operational center for modeling technology will leverage existing programs and provide feedback to ongoing research programs.
APPROACH: The Agency's Center for Exposure Assessment Modeling (CEAM) will work with the regions and ATSDR to identify support needs, conduct site-specific assessments, and provide continued technical support. Modeling software, users manuals, data bases, and procedural handbooks will be developed, distributed, maintained and supported. Case studies will be conducted with emphasis on multi-media assessments and associated uncertainties. Results will be used for technology transfer and as a basis for additional research.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

NO PROJECT STATUS TEXT AVAILABLE

STATUS AND SCHEDULE OF DELIVERABLES:

NO REFERENCES IN DELIVERABLES FILE FOR THIS PROJECT

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