

United States  
Environmental Protection  
Agency

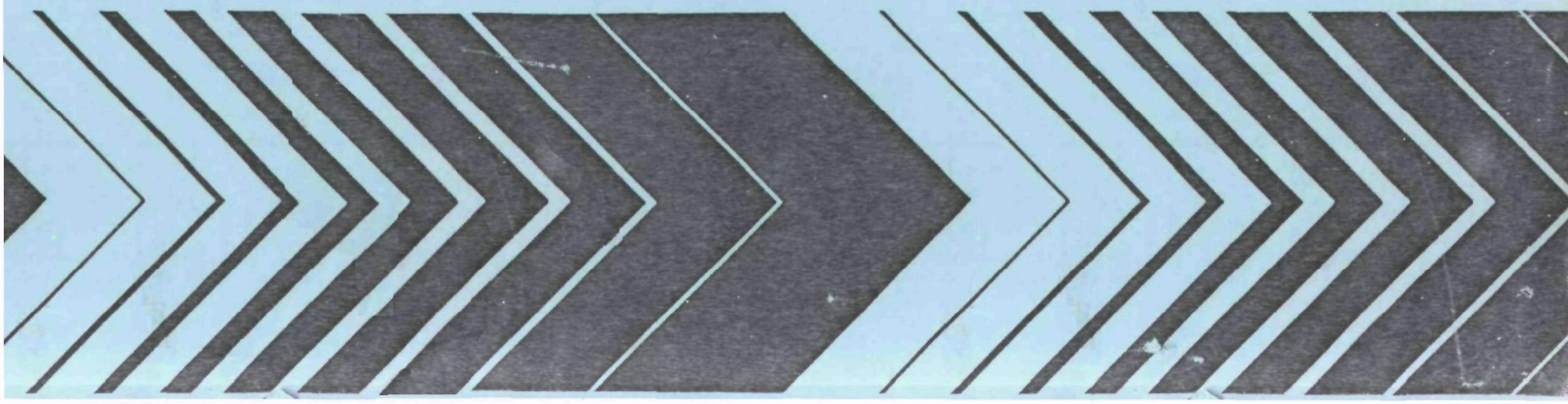
October-December  
1988

Research and Development

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# **EPA Research Report**

**Environmental  
Research  
Laboratory  
Athens, GA 30613**



FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: A101 AIR  
ISSUE: F Stratospheric Ozone  
PPA (L): 75 STRATOSPHERIC OZONE

PPA (S): STRATOSPHERIC OZONE  
RC: K ERL ATHNS

PROJECT: 42 Stratospheric Ozone Modification

PROJECT OFFICER: R. G. Zepp

PHONE: FTS-250-3428

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PLANNED START: 10/01/88 PLANNED END: 09/30/94

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PROJECT DESCRIPTION:

GOAL: Develop reliable methods of estimating the harmful exposure of ecosystems to UV-B radiation received under current & projected climatological conditions.

RATIONALE: Evaluation of risk to ecosystems posed by decreased strat. ozone requires ability to estimate current & future expected doses of UV-B under different scenarios. Estimation procedures must account for physical dependencies & variations in concentrations of UV-B absorbing species in the environment as well as action spectra for harmful UV-B effects.

APPROACH: Existing models will be modified to evaluate effects of decreased strat. ozone on UV-B exposure rec'd by organisms at land surface and in aquatic ecosystems. Models will be developed to estimate transport effects on UV-B exposure in aquatic ecosystems & effects of UV-B on geochemical cycles.

These models will be field tested to evaluate their accuracy & to correct any deficiencies that may be revealed. This will be accomplished by measurements of solar irradiance reaching the ground under a variety of atmospheric conditions, & by experimental & field work to test & improve the estimation methods for hydrospheric transmissivity as a function of the concentration of light-absorbing constituents.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

0.5 FTE was allocated to ERL-Athens in FY89 for project 42. Inhouse work has begun on exposure assessment methodologies.

Activities during the quarter included the initiation of research on the development of an appropriate UV-B chemical actinometer for evaluating exposure model predictions of solar UV-B irradiance reaching the earth's surface and downwelling into aquatic ecosystems. Systems examined included actinometers based on the photoreactions of two ketones, valerophenone and 2-pentanone, in water. Quantum yield and temperature studies were initiated during the quarter. Results indicate that both actinometers may be very useful. Each has

a reaction quantum yield near unity with virtually no temperature dependence between 10 and 40 degrees C. For comparison, the temperature dependence for direct photolysis of the actinometer p-nitroanisole also was examined during the quarter; this photoreaction also was found to be little affected by temperature changes.

Dr. Richard Zepp presented a paper on "Consequences of Stratospheric Ozone Depletion: Actinometers for Evaluating Integrated UV-B Exposure" at the Annual Meeting of the Society of Environmental Toxicology and Chemistry, Washington, DC in November.

No R&D funds have yet been authorized for expenditure by ERL-Athens on project 42. Plans are being made, however, to fund an inhouse contract to provide laboratory personnel support, and to conduct a workshop on UV-B effects on geochemical processes in aquatic and terrestrial ecosystems, probably to be held next spring at Woods Hole Oceanographic Institute.

Planning for a field program to test our current models of light transmission in the hydrosphere, to be initiated during the spring in area lakes, was begun this quarter. Personnel were identified and recruited, and general project objectives outlined.

A currently used model of UVB transmission in the atmosphere (developed at the University of Chicago) was acquired and implemented on the Wyse workstation. Analysis of this model will help define the upgrade path for the EXAMS atmospheric transmission model and may indicate some alternative models for additional study. In preparation for expansion of the EXAMS program to accommodate UVB exposure analysis during this quarter, the suite of EXAMS implementations that had been developed to accommodate machine-specific features of the various supported platforms (DSI board, MS-DOS, VAX, Siemens computers) were integrated into a single code set. This was accomplished primarily by converting machine-dependent input/output routines into Fortran run-time formats controlled by datasets that incorporate the results of an analysis of the relevant machine dependencies.

#### STATUS AND SCHEDULE OF DELIVERABLES:

- |      |  |          |            |
|------|--|----------|------------|
| 8219 | DUE: 06/30/89  | REVISED: | COMPLETED: |
|      | Report: Assessments of UV-B effects on photochemical transients in aquatic and terrestrial ecosystems.                             |          |            |
| 8220 | DUE: 09/30/89  | REVISED: | COMPLETED: |
|      | Report: The Scientific Assessment of Existing Mathematical Models for Exposure of Terrestrial and Aquatic Biota to UV-B Radiation. |          |            |

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ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: A101 AIR  
ISSUE: G 2  
PPA (L): 94 Ecological Effects of Global Climate Change  
  
PPA (S): Ecol. Glo. Climate  
RC: K ERL ATHNS  
PROJECT: 34 Effects of Climate Change on Physicochemical Processes  
PROJECT OFFICER: Richard G. Zepp PHONE: FTS-250-3145

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PLANNED START: 04/01/89 PLANNED END: 09/30/98

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PROJECT DESCRIPTION:

GOAL: Develop physicochemical process models to describe effects of climate changes on emissions and dry deposition of greenhouse gases.

RATIONALE: Long-term climate changes will have important effects on the various physicochemical processes affecting natural emissions and dry deposition of radiatively important gases in land and water. Even small increases in flux of natural emissions may induce significant effects on global climate. Process models and kinetic and equilibrium data are needed to assess such effects under various climate scenarios.

APPROACH: Develop models for volatilization, sorption, chemical reactions and photochemical reactions involved in the natural emission and deposition of radiatively important gases. Physical process studies include partitioning between air and water, and water and soil, plus volatilization from water and soil. Temperature effects and, for soils, moisture and composition will be included. Chemical studies will focus on mechanisms and decay rates of ozone. Effects of temperature and factors such as pH and chemical composition will be examined. The influence of photochemical processes (rates and mechanisms) will be determined. Trace metal, pH, and humic effects, and soil composition and origin will be included in developing relationships and models.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

No FTE's were allocated to ERL-Athens for this project for FY89, and no R&D funds have yet been authorized for expenditure. Plans are being made, however, for both inhouse and extramural research once resources are available.

STATUS AND SCHEDULE OF DELIVERABLES:

NO DELIVERABLES AVAILABLE



FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
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CODE TITLE

BUDGET SUB-ACTIVITY: A101 AIR  
ISSUE: G 2  
PPA (L): 94 Ecological Effects of Global Climate Change  
  
PPA (S): Ecol. Glo. Climate  
RC: K ERL ATHNS  
PROJECT: 36 Biogenic Production of Nitrous Oxide and Methane in the Env.  
PROJECT OFFICER: David Lewis PHONE: FTS-250-3358  
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PLANNED START: 04/01/89 PLANNED END: 09/30/98  
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PROJECT DESCRIPTION:

GOAL: Elucidate the relative contributions of bacterial production of nitrous oxide and methane among different environments (wetlands, soils, etc.), and the environmental factors affecting the production rates.

RATIONALE: Nitrous oxide and methane, major products of microbial metabolism, have great potential for adversely affecting the global climate. Global monitoring data indicate significant shifts in ambient concentrations of these gases in the atmosphere; therefore, an improved understanding of microbial production and of transformation of these gases is needed to provide capabilities for predicting future global climatic changes and guiding resource management.

APPROACH: A group of experts will be convened in a workshop to arrive at a consensus concerning which ecosystems and environmental parameters merit the highest research priority. Laboratory and field studies will be conducted to elucidate which microorganisms and environments most significantly contribute to nitrous oxide and methane production, and what rate-limiting processes and environmental parameters most critically affect gas production rates.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

We have reviewed the literature, and formulated tentative research plans regarding biogenic contributions of nitrous oxide. The organization of a workshop, and subsequent pursuance of high priority research topics awaits funding of this task.

Recent research indicates that radiatively important trace gases other than carbon dioxide are also likely to influence global climate changes significantly. These gases include methane, nitrous oxide, and tropospheric ozone. In addition, carbon monoxide (CO), although not itself radiatively important, has significant effects on the atmospheric concentration of methane and tropospheric ozone.

The atmospheric concentrations of these gases are regulated, in part, by chemical and biological processes that occur in the biosphere. Microorganisms in terrestrial and aquatic ecosystems produce large quantities of methane and nitrous oxide. Carbon monoxide is produced through chemical and photochemical oxidation of natural organic matter in natural water bodies. In addition, methane, nitrous oxide, and carbon monoxide are metabolized by microbiota and ozone is removed from the troposphere through reactions with vegetation, soil, and natural water.

Our research focuses on developing generalizable mathematical relationships that can be used to model the effects of climate changes on biological and geochemical processes that are important sources and sinks of methane, nitrous oxide, carbon monoxide and tropospheric ozone in terrestrial and aquatic ecosystems. The results are used in terrestrial and aquatic systems level mathematical models to predict the net fluxes of these gases as a function of various hypothesized land use or climate scenarios. These studies will provide improved capabilities to determine both current and potential global contributions of biogeochemical versus anthropogenic sources of these trace gases as well as to evaluate the effects of various remediation options.

We will discuss our current research efforts to provide a better assessment of contributions of microbial activities to global nitrous oxide, methane, and carbon monoxide concentrations through an improved understanding of (1) the relative significance of different environments as sources and sinks and (2) the environmental factors affecting production rates of these trace gases, and well as our research efforts to improve the understanding of the geochemical processes in land and water on the production, decay, and biosphere-troposphere exchange of carbon monoxide, ozone, methane, and nitrous oxide.

An abstract, "Sources and Sinks of Radiatively Important Trace Gases in the Biosphere" (Rogers, Burns, Zepp and Lewis), was submitted upon invitation for presentation at the 1989 annual meeting of the Air and Waste Management Association, June 25-30. Dr. Rogers will present the paper.

#### STATUS AND SCHEDULE OF DELIVERABLES:

8232 DUE: 07/31/89 REVISED: COMPLETED:  
Report: Microbial processes that influence emissions of radiatively important gases



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CODE TITLE

BUDGET SUB-ACTIVITY: B101 WATER QUALITY  
ISSUE: A WQBA/PERMITTING  
PPA (L): 10 WASTELOAD ALLOCATION MODELING AND SUPPORT

PPA (S): WASTELOAD ALLOCATION  
RC: K ERL ATHNS

PROJECT: 06 Environmental Process Characterization

PROJECT 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 role of inorganics in pollutant transformation by photolysis and the kinetics of redox reactions are inadequately understood for reliable use in exposure assessment models. Sorption of ionizable organics also significantly affects pollutant transport. Toxic metal speciation and transport needs further investigation since metal toxicity depends upon the species.

APPROACH: Using natural waters, sediments and reference materials, equations for the kinetics of materials will be tested. 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. Studies will examine effects of inorganics on photochemistry, biotic influences on redox reactions in abiotic systems, binding characteristics of metals and humics, and sorption processes of ionizable organics on sediments. Distribution coefficients of metals will be determined for various solid substrates.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Research was continued on the influence of light on the oxidation of organic substrates by manganese oxides. Kinetic studies of the oxidation of p-chlorophenol were conducted using monochromatic radiation corresponding to the maximum absorption of manganese dioxide (336 nm). The pH dependence of the oxidation rate of p-phenylphenol in manganese oxide suspensions exposed to sunlight also was investigated. Studies of the influence of light on the oxidation of anilines by manganese oxides were initiated; the oxidation of p-chloroaniline was examined. Work on the photoredox reactions of copper was also continued. Quantum yields were determined as a function of pH for the



photoreduction of copper (II) complexed by nitrogen ligands. Kinetic studies were conducted in sunlight for comparison. Two journal articles were submitted for publication during the quarter: "Hydrogen Peroxide Decay in Waters with Suspended Sediments: Evidence for Biologically Mediated Processes" and "Aquatic Humic Substances as Sources and Sinks of Photochemically Produced Transient Reactants."

Studies of the effects of pH on the adsorption of anionic organic compounds to sediments have been initiated. Titration of a well characterized sediment using a pH-stat constructed here has shown that, between the ambient pH value of 7.8 to approximately pH 5.5, hydrogen ion activity can be controlled by the addition of acid (HCl) to within about 0.5 units. Titration of pentachlorophenol (PCP, pKa equal to 4.8) between pH values of 7.8 and 4.0 in EPA 11 sediment (10 g sediment in 200 ml water) shows the concentration of pentachlorophenol in the aqueous phase to range from 80% of total added (at pH 7.8) to approximately 4% (at pH 4.0). Between pH values of 3 and 4 no difference was observed in the partition coefficient. This is highly consistent with octanol-water partitioning data for PCP in the same pH ranges. Further studies controlling the pH at higher values with the addition of base (NaOH) are anticipated, along with titration of other compounds having different properties.

A paper on the homogeneous hydrolysis rate constants for selected chlorinated methanes, ethanes, ethenes and propanes has been drafted. This paper contains alkaline hydrolysis rate constants and activation parameters for 15 chlorinated hydrocarbons. The data will provide a basis for developing a structure reactivity relationship for estimation of rate constants for other halogenated hydrocarbons. A draft journal article entitled "Hydrolysis of Chlorostilbene Oxide II. Hydrolysis in Aquifer Samples and in Sediment-Water Systems" contains results that provide support for a model that quantitatively describes abiotic hydrolysis in heterolytic systems.

Kinetic studies of the degradation of Solvent Red 1 in anaerobic sediment-water systems show that the disappearance of the dye followed pseudo-first-order kinetics over two half-lives. The half-lives in two sediments were 94.6 and 67.9 hours.

Studies progressed on the degradation of diphenyl- and dialkyl-N-nitrosoamines in anaerobic sediments. While diphenyl-N-nitrosoamine was degraded to diphenylamine with a half-life of 11.8 h, diethyl-, dipropyl-, and dibutyl-N-nitrosoamines were stable over a period of 14 days. Sorption studies indicate the dialkyl-N-nitrosoamines do not sorb to the sediment and that the diphenyl-N-nitrosoamine is only weakly sorbed. These results indicate that the dialkyl-N-nitrosoamines will be persistent and highly mobile in groundwater environments.

#### STATUS AND SCHEDULE OF DELIVERABLES:

8149 DUE: 06/30/89 REVISED: COMPLETED:  
Report: Sorption Processes for Ionizable Organics on Sediments.

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CODE TITLE

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

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

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PROJECT DESCRIPTION:

GOAL: Test the predictive accuracy and determine the applicability of microbial transformation rate coefficients for water quality models and evaluate bioaccumulation of toxicants in aquatic organisms in relation to thermodynamic equilibrium processes.

RATIONALE: This research is required to produce a reliable approach for predicting biologically mediated accumulation and degradation of pollutants to improve water quality and risk assessment models.

APPROACH: Rate coefficients for microbial transformation of xenobiotic chemicals will be determined using microbial populations collected from lakes and streams. Bioaccumulation in organisms of varying size and lipid content and of different species will be determined using toxic chemicals that have 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:

One paper, "Special applications of insect gut microflora in kinetic studies of microbial substrate removal rates" (Lewis & Said) was accepted for publication in the Journal of Environmental Toxicology and Chemistry. Laboratory microcosm studies regarding nitrification rates have been described in a manuscript "Nitrification by attached bacteria in an aquatic ecosystem" (Said, Lewis, Holm & Kollig), which is being internally reviewed.

STATUS AND SCHEDULE OF DELIVERABLES:

8150 DUE: 08/31/89 REVISED: COMPLETED:  
Internal report on microbial process highlights.



PRINT DATE: 01/30/89  
PMS-060

CLIENT OFFICE OWRS

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: B101 WATER QUALITY  
ISSUE: A WQBA/PERMITTING  
PPA (L): 10 WASTELOAD ALLOCATION MODELING AND SUPPORT

PPA (S): WASTELOAD ALLOCATION  
RC: K ERL ATHNS

PROJECT: 19 Wasteload Allocation Modeling and Support

PROJECT OFFICER: Tom Barnwell

PHONE: FTS-250-3210

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

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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:

Cooperative researchers at Tufts University revised a paper, "DO Model Uncertainty with Correlated Inputs," based upon reviewer comments and resubmitted it to the Journal of the Environmental Engineering Division. Continuing work on graphical presentation of uncertainty information is complete and a master's thesis describing the work is in preparation.

Cooperative researchers at Cornell University continue to make good progress with the CORMIX model. Funding was received this quarter from the Office of Water to complete work on this project. Links between program models were completed this month and model validation, including calibration of

coefficients, has begun. Abstracts have been submitted for the 1989 ASCE Hydraulics and Environmental Engineering Division summer conferences and for the International Association for Hydraulic Research Congress. Additional funding was received to incorporate the work in a short course this summer.

A LOTUS spreadsheet model was developed to reproduce the calculations by the Environmental Defense Fund in their paper "Polluted Coastal Waters: The Role of Acid Rain." A seminar reviewing procedures used in the report was presented.

Testing, preparation of code, composition of support documentation, and master file/diskette creation for the distribution version of WASP for VAX and PC systems for release 4.14 is in progress.

Allen Medine conducted the course "Metal Contamination in Surface Waters: Methods for Assessment and Control" for Region 8 and states December 13-14 in support of the 304(1) program. Max Dodson, Region 8 Water Management Division Director, sent a memo of thanks, declaring the workshop a success.

We continued migration of CEAM model distribution and registered user data base from VAX to PC environment. We also began implementation of a CEAM database for all CEAM training and model distribution activities. Initial preparation of CEAM's FY89 training courses began including selection of tentative dates, course descriptions, and venues. Five courses are planned this summer including:

- QUAL2E with Uncertainty Analysis	July 10-14
- Exposure and Bioaccumulation Models	July 24-28
- MINTEQ	August 22-24
- Estuarine Wasteload Allocation	September 11-15
- RUSTIC	September 18-22

#### CEAM BBS and Model Distribution Statistics

BBS Statistics:	Total Calls	477
	New Users Added	70
	Total Uploads	14
	Total Downloads	270

#### Model Distribution:

Model	Diskette	BBS	Tape
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WASP4	27	16	0
SWMM3	15	4	0
HSPF9	23	0	3
MINTEQ	57	3	1
QUAL2E	44	6	1
DYNTOX	10	7	0
EXAMSII	20	3	2
PRZM	16	11	3
LC50	5	6	0
SARAH	9	1	0

FGETS	13		1		0	
GCSOLAR	7		3		0	
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TOTAL	246	+	61	+	10	= 317

STATUS AND SCHEDULE OF DELIVERABLES:

7851 DUE: 07/31/88 REVISED: 07/31/89 COMPLETED:  
Report on Expert Advisor for CORMIX Model

2/88 - delay to 7/89 a result of FY-88 Congressional Budget  
actions; 5/88 - transferred from B-101 A-15 during FY-89  
PPA devel. process and title change





FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
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ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

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

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

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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. Chemical and microbiological process characterization studies will also be conducted to elucidate the transformation and transport of metals and organics in surface and subsurface environments.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Dr. George Bailey attended the International Symposium on Environmental Life Elements and Health, November 1-5, 1988, in Beijing China. He and Mr. Lin Yuhuan each presented a scientific paper. Two manuscripts were submitted for publication in the symposium proceedings. Dr. Bailey presented seminars at the Research Center for Eco-Environmental Sciences, Chinese Research Academy of Sciences, Beijing; the Chinese Research Academy of Environmental Sciences, Beijing and Shaanxi, and the Environmental Protection Bureau (National Environmental Protection Agency), Xian. Dr. Bailey presented a third paper based on Mr. Lin's work at the American Society of Agronomy (ASA) National Meeting, Anaheim, California, November 27-December 2, 1988.

**Titles of manuscripts/presentations are:**

**"Metal Interactions at Sulfide Mineral Surfaces: Part II. Adsorption and Desorption of Lanthanum," Lin Yuhuan, George W. Bailey and Alan T. Lynch (presented and submitted for publication in Symposium proceedings).**

**"Metal Interactions at Sulfide Mineral Surfaces: Part III. Metal Affinities in Single and Multiple Ion Adsorption Reactions," Lin Yuhuan, George W. Bailey and Alan T. Lynch (presented and submitted for publication in Symposium proceedings).**

**"Metal Interactions at Sulfide Mineral Surfaces: Part IV. Adsorption and Precipitation Reactions," Lin Yuhuan, George W. Bailey and Alan T. Lynch (presented at ASA National Meeting).**

**STATUS AND SCHEDULE OF DELIVERABLES:**

**8152 DUE: 09/30/89 REVISED: COMPLETED:**  
**Internal Report: Joint US-PRC Studies on Pollutant Transformation Processes, Metals Speciation and Assessment Models.**

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
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ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

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

PPA (S): TOXICS IDENT.  
RC: K ERL ATHNS

PROJECT: 02 Identify and Compile Data on Occurrence of Organics

PROJECT OFFICER: John M. McGuire PHONE: FTS-250-3185

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PLANNED START: 10/01/82 PLANNED END: 09/30/92

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PROJECT DESCRIPTION:

GOAL: Identify and determine distribution of unlisted chemicals in industrial wastewaters. Compounds identifiable by empirical mass spectra matching and those eluding identification by this technique will be included.

RATIONALE: As new industrial technology is implemented, different chemicals are introduced to wastewaters. Lists of regulated chemicals must be continually updated, otherwise the listing may contain compounds that occur infrequently and not contain other hazardous or toxic chemicals that, in fact, may occur more frequently. Determining the distribution of unlisted hazardous and toxic chemicals will permit maintenance of relevant 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. 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:

As reported last quarter, one list of target compounds for confirmation and another for multi-spectral identification of hits and misses have been generated from the study of POTW and organic industry GC/MS tapes from the Industrial Technology Division. Due to the last minute arrival of retained extracts from 10 samples, the list is being reconsidered before final multi-spectral analysis is completed.

STATUS AND SCHEDULE OF DELIVERABLES:

7579 DUE: 12/30/88 REVISED: 11/30/89 COMPLETED:  
Report on Multi Spectral Identifications of MIS LIB Compounds. (K)

2/88 - delay to 11/89 a result of FY-88 Congressional Budget actions



PRINT DATE: 01/30/89  
PMS-060

CLIENT OFFICE ODW

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: C104 DRINKING WATER  
ISSUE: F GROUNDWATER  
PPA (L): 82 Ground Water Methods, Information Transfer & Applications  
PPA (S): GW MTHDS, INFO, & APPL  
RC: K ERL ATHNS  
PROJECT: 22 Identify Unlisted Contaminants in Potential DW Sources  
PROJECT OFFICER: John McGuire PHONE: FTS-250-3185

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

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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 that pose a health risk in drinking water. 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 analyses of groundwater and other potential DW sources to identify 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:

The ether extracts of the pilot plant chlorination referred to last quarter showed the concentrations of most analytes to be too low for effective use of GC/FT-IR. One GC peak present as a moderate level and corresponding to one of the unidentified, unchlorinated compounds in earlier Risk Reduction Engineering Laboratory studies was examined by GC/FT-IR, but no definite conclusions could be reached concerning its structure.

STATUS AND SCHEDULE OF DELIVERABLES:

8117 DUE: 08/31/90 REVISED: COMPLETED:  
Report: Ozonation Products of Drinking Water.



PRINT DATE: 01/30/89  
PMS-060

CLIENT OFFICE OSW

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS

Office of Environmental Processes and Effects Research

ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: D109 HAZARDOUS WASTE  
ISSUE: C WASTE CHARACTERIZATION  
PPA (L): 28 LAND DISPOSAL ASSESSMENT & EVALUATION OF OTHER MGMT SYSTEMS  
  
PPA (S): LAND DISPOSAL ASSESS  
RC: K ERL ATHNS  
PROJECT: 03 Determine Chemical Transformation Pathways and Rates  
PROJECT OFFICER: Jackson Ellington PHONE: FTS-250-3197  
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PLANNED START: 10/01/85 PLANNED END: 12/31/99  
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PROJECT DESCRIPTION:

GOAL: Prepare transformation pathway profiles of RCRA regulated chemicals in order to provide data for environmental risk assessments.  
RATIONALE: Under Subparts B and C of RCRA Part 261, listed chemicals are being evaluated for their potential hazard to the environment when improperly treated, stored, transported or disposed of. The chemicals already listed under Subpart B are being subjected to mathematical modeling to determine acceptable concentrations in leachates for each listed chemical and its transformation products. Unlisted chemicals are being similarly evaluated under Subpart C as candidates for listing. Assessments of concentrations resulting from anticipated environmental conditions are necessary in order to determine acceptable leachate concentrations.  
APPROACH: Transformation processes, products and rates will be evaluated on a theoretical basis to identify those that are likely to be significant. When the evaluation indicates a need for experimental confirmation of reaction rates or transformation products, appropriate experiments will be conducted. Results of the theoretical considerations and laboratory experiments will be published as transformation pathway profiles.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A Research Brief was drafted entitled "Pathway Analysis of Chemical Hydrolysis for 14 RCRA Chemicals." The brief identifies the pathway profiles of hydrolysis, the intermediate and/or final products and rates of hydrolysis (including references) of parents and intermediate products. A preliminary report of the pathway analysis was provided to OSW.

Laboratory measurement of second-order acid hydrolysis rate constants for seven substituted acetanilides are in progress. The rate constants will be correlated with molecular spectroscopic properties to determine property-reactivity correlations.



Dr. Ellington chaired a session on the RCRA/Superfund: Toxics Monitoring Symposium at the Southeast Regional American Chemical Society Meeting held in Atlanta on November 9-11, 1988.

An attempt was made to determine the photolysis product of N,N-diphenyl nitrosamine in water. Due to possible instrumental effects, the compound was identified as either 9-nitroso-9H-carbazole or 9H-carbazole. The uncertainty is due to the fact that the nitroso compound would decompose to the carbazole at the temperature of the GC injection port.

Two peaks from hydrolysis of 1,2-dichloroethane were identified. One was identified as hydrogen chloride and the other ethylene glycol.

The identities of 16 compounds to be used in degradation studies were confirmed by mass spectrometry.

Hydrolysis products of phorate and phorate sulfoxide were identified. The phorate sample showed both phorate and diethyl sulfide; the sulfoxide sample showed no sulfoxide and only very small peaks corresponding to alkyl sulfides and thiols. None of the observed compounds seems a likely hydrolysis product of either phorate or of the phorate sulfoxide.

#### STATUS AND SCHEDULE OF DELIVERABLES:

7950	DUE: 06/30/89	REVISED:	COMPLETED:
	Report on Hydrolysis Rate Constants for Enhancing Property-Reactivity Correlations.		

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: D109 HAZARDOUS WASTE  
ISSUE: C WASTE CHARACTERIZATION  
PPA (L): 28 LAND DISPOSAL ASSESSMENT & EVALUATION OF OTHER MGMT SYSTEMS  
  
PPA (S): LAND DISPOSAL ASSESS  
RC: K ERL ATHNS  
PROJECT: 07 Environmental Process Characterization - Metals  
PROJECT OFFICER: Arthur W. Garrison PHONE: FTS-250-3145  
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PLANNED START: 10/01/84 PLANNED END: 12/31/99  
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PROJECT DESCRIPTION:

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

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

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. Distribution coefficients will be determined using plasma emission spectroscopy. Metal-ligand interactions will be studied using laser spectroscopy. Kinetic equations and equilibrium constants will be determined for use in exposure and risk models. Measurement, distribution, and significance of redox potential of aquifer systems will be studied.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Major progress has been achieved by our University of Georgia cooperators in their application of a Gaussian distribution model for competitive metal binding with dissolved organics to fit their Lanthanide ion probe spectroscopic titration data. The paper "Characterization of Metal Binding Sites in Humic Acids by Lanthanide Ion Spectroscopy" was accepted for publication in Analytical Chemistry, and a draft of another, "A Study of the Competitive Binding of Protons and Metal Ions in Fulvic Acids by Lanthanide Ion Spectroscopy," is currently undergoing final revision before submission for journal publication. Currently, a draft of a paper on the binding of aluminum by dissolved organics in natural waters is being prepared. At ERL-Athens, Lanthanide ion probe titration spectroscopy has been used successfully to study the binding of lead by dissolved organic matter.

Georgia Institute of Technology (GIT) cooperators have completed the major portion of their matrix titration experiments using total dissolved organic

matter from the Suwannee River (SRDOM), carried out at three different ionic strengths. These data are needed to completely characterize the proton binding properties of SRDOM. This information is essential for application of the Gaussian distribution model to the study of competitive metal binding. These cooperators also have successfully isolated a substantial quantity of SRDOM by the reverse osmosis technique they developed last year. About 10 grams of SRDOM was give to ERL-Athens for use in our metal-organic binding studies.

The possibility of incorporating a metal-organic complexation component into MINTEQ, the metal speciation model currently used for exposure assessment of toxic metals by OSW, was discussed at a joint meeting of UGA, GIT, and ERL-Athens cooperators in December. There was a consensus that development of an algorithm for this component is quite achievable and should be the immediate focus of the cooperators.

pH-dependent cationic adsorption profiles for six aquifer material samples were completed this quarter. At present, modeling the adsorption of anionic species to aquifer materials is unsatisfactory. Hence, additional experimental work soon will begin using individual ionizable species. In December, 30 aquifer material samples were collected at the joint ERL-Athens/USGS field testing site near Globe, AZ for further studies of metal-metalloid adsorption on aquifer solids. Four out of five attempted well installations at this site were successful.

A methodology has been developed using orthogonal functions for deconvoluting mixed emission spectra on the ICP. In addition, preliminary work on salt concentration effects on ICP nebulizer efficiency has led to the implementation of a scandium internal standard procedure in the ICP analytical protocol. Previous dilution procedures often led to significant sensitivity losses.

Work also has been completed on a cation exchange resin preconcentration procedure for measuring contaminant concentrations at background levels in groundwater.

Technical assistance (in conjunction with the ERL-Athens Assessment Branch) was provided to: 1) Ed Bates (ERL-Cincinnati), Big 5 Wetlands Project, and 2) EPA Risk Assessment Forum, on use of MINTEQA2 as a tool for investigating the potential bioavailability of metals, especially lead.

Work continues at the University of Guelph on desorption of various metals found on bacterial cell walls and cell wall-clay complexes. A draft manuscript entitled, "Immobilization of Metallic Ions by Escherichia coli Envelope and Bacillus subtilis wall - clay Mixtures" is undergoing internal review and clearance. Preliminary work has started at the University of Arkansas on metal sorption--Cu(II), Cd(II), Ag(I) and La(III)--by three fungi:Aspergillus niger, Rhodotorula ulzamae and Saccharomyces cerevisiae.

#### STATUS AND SCHEDULE OF DELIVERABLES:

- |      |   |          |            |
|------|---|----------|------------|
| 8157 | DUE: 08/31/89   | REVISED: | COMPLETED: |
|      | Comprehensive Report on Applying Electrostatic Adsorption Theory to Natural Systems |          |            |
| 8158 | DUE: 03/31/89   | REVISED: | COMPLETED: |
|      | Report Defining Metal Complexation/Chelation Sites in Humic Materials               |          |            |

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CODE TITLE

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

PPA (S): LAND DISPOSAL ASSESS  
RC: K ERL ATHNS

PROJECT: 17 Environmental Process Characterization (Biological)

PROJECT OFFICER: John E. Rogers PHONE: FTS-250-3592

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

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PROJECT DESCRIPTION:

GOAL: Provide integrated (multimedia) methods and data for implementing the Hazardous Waste Management Amendments, including evaluating waste management and treatment needs based on potential human health and environmental impacts. RATIONALE: Current regulatory activities including, RCRA Reauthorization requirements relative to land disposal evaluation, are demonstrating the lack of consistent methods and data for determining the health and environmental impact of various regulatory options. Integrated (multimedia) methods that accommodate knowledge of uncertainty are needed for more accurate and consistent decision-making on waste management options. APPROACH: Mechanisms of anaerobic biotransformations of xenobiotic chemicals will be characterized using kinetic concepts. Laboratory studies will be conducted to test these models and to identify environmental parameters that affect the rates and extent of the biotransformation processes.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

The effects of the composition of headspace gas on the degradation of 2,4-dichlorophenol (DiCP) in anaerobic sediments were observed. Reaction bottles containing 10 ml of sediment/water slurry (1g dry sediment to 10 ml water) were amended with 10 mg/l of 2,4 DiCP. The initial headspace compositions were H2/N2 (5%/95%), CO2/N2 (5%/95%), N2 (99.9%) or compressed air. Two experimental approaches were used. In the first, the headspace gas was periodically exchanged with the initial gas composition during the incubation period and in the second the headspace gas was not exchanged over the entire incubation period. The degradation rate was greatest in sediments in which the headspace composition was exchanged. In these studies, degradation of 2,4 DiCP was complete by day 10 for CO2/N2 and air and by day 14 for H2/N2 and N2. In reaction bottles in which the headspace was not exchanged, 2,4 DiCP was absent in CO2/N2 after 14 days and present in sediments with headspace of air or N2 after 17 days and in H2/N2 headspace bottles after 28 days. The results

indicate that in all treatments the methane production reached an exponential level before 2,4 DiCP degradation began.

Reductive dechlorination of dichlorophenols was investigated in pond sediments from two sites in the Athens area. Fresh Cherokee Pond sediment dechlorinated 2,4- and 3,4-dichlorophenol to monochlorophenols within 31 days, whereas fresh Bolton's Pond sediment dechlorinated 2,3-, 2,4-, and 2,6-dichlorophenol to monochloro- products after approximately 17, 12, and 41 weeks, respectively. Adapted Cherokee Pond sediments dechlorinated 2,4- and 3,4-dichlorophenol within 4 days, whereas Bolton's Pond sediment was significantly slower, dechlorinating the 2,3-, 2,4-, and 2,6-dichlorophenol isomers within 3, 2, and 4 weeks, respectively. When 2,3-, 2,4-, 2,5-, 2,6-, 3,4-, and 3,5-dichlorophenol were added individually to subsamples of the adapted sediments from both sites, differences in monochloro- products and dechlorination rates were observed. The differences in adaptation, product formation, and dechlorination rate appear to be site specific.

The following two abstracts were submitted for the 1989 ASM Meeting to be held in New Orleans, LA, in May: (1) Effect of Gas Phase Composition on Anaerobic Biodegradation of 2,4-Dichlorophenol (Howard, Hale & Struijs), (2) A Comparison of the Reductive Dechlorination of Dichlorophenols in Fresh and Acclimated Sediments from Two Ponds (Hale & Rogers).

Laboratory experiments on the microbial degradation rates of methyl - chlorobenzoate, methyl parathion, and 2,4-D butoxyethyl ester relative to a benchmark chemical, 2,4-D methyl ester, have been completed. Kinetic data were obtained using biofilm, water, and sediment samples (separately) collected from field sites in Georgia and Florida. Degradation rates varied widely, depending on the test chemical and environmental sample. However, degradation rates relative to the benchmark chemical degradation rates were constant. These data will be used in a journal article "Microbial substrate removal rate coefficients relative to a benchmark chemical" (Newton, Lewis, Gattie).

The UGA cooperative agreement has not been funded; therefore, we have no progress to report on our planned research on microbial adaptation to chemical degradation (Hodson) or biofilm species composition effects on microbial degradation and nutrient cycling (Shotts).

#### STATUS AND SCHEDULE OF DELIVERABLES:

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

3/87-transf. from Ada to Athens to correct mistake on FY-87  
final version PPA's; 5/87-due date revised as a result of  
reprogramming of HW R&D resources to Wetlands program during  
FY-88 PPA planning process

8163 DUE: 04/30/89 REVISED: COMPLETED:  
Report on Evaluating the Utility of Current Methods for Estimating Anaerobic  
Degradation Rates for Use in Evaluative Models

6/88 - moved from Y-105 B-02/33 to D-109 C-28/17

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CODE TITLE

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

PPA (S): LAND DISPOSAL ASSESS

RC: K ERL ATHNS

PROJECT: 21 Multimedia Modeling with Uncertainty Analysis

PROJECT OFFICER: Lee A. Mulkey

PHONE: FTS-250-3160

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

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PROJECT DESCRIPTION:

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

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

APPROACH: The regulatory modeling system under development by OSW will be enhanced, tested, and further developed to produce a comprehensive multimedia exposure assessment system. A major part of this approach will include data analysis, monte carlo programming, and error analysis to derive uncertainty estimates. Field testing and case study applications will be completed to further evaluate uncertainties.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Dr. Dave Brown, Dr. Nick Loux, Jerry Allison, Terry Allison and Lee Mulkey developed metal speciation and transport modeling results for lead from soils to human gastrointestinal tracts. Dr. Brown presented the results at the Risk Assessment Forum Colloquium on Assessing Bioavailability of Lead and Other Metals December 7 and 8 in Washington, DC. The effort was well received by the Colloquium attendees and will be followed-up with an outline of the effort that would be required to implement such an approach as part of the overall risk assessment scenario for lead in soils. If implemented, this project should substantially reduce the uncertainties inherent in current risk assessment procedures.

Effort this quarter in direct support of OSW's development of a new rule for waste characteristics included the development of a new plan for research and model development activities geared for developing proposed regulations for metals by December 1989 and promulgating final rules by July 1990. Dr. Brown and Dr. Loux met with headquarters OSW technical staff December 8 to discuss model development issues. A joint planning meeting in Athens is planned for February 2 and 3 to finalize model development plans.

A series of four additional monitoring wells were installed at the Globe, AZ mine waste site involved in our EPA/USGS cooperative efforts for obtaining data sets to test the MINTEQA2 metal speciation/transport model. Core samples from the bore holes were collected and returned to ERL-Athens for characterization.

Other OSW modeling support activities included:

- o Development and testing of an overlaid version of the Multimedia Model for execution on PC.
- o The EPA CML code was modified to meet needs of the OSW transient case modeling project and a series of modeling runs was completed for conservative chemicals to be covered in the next round of rule making. Results of these exercises will be incorporated in the upcoming rule.
- o Extensive modeling runs were completed for G. Michaels of the Economic Analysis Branch OPA/OPPE to help evaluate the impact of the upcoming rule on the pulp and paper industry.
- o A new version of MINTEQ (MINTEQA2) was released for distribution. The new code was first used in the context of the MINTEQA2 course presented in Boulder, CO during September. It incorporates updated sorption algorithms and a substantially revised preprocessor code (PRODEFA2). The new sorption algorithm, based on the diffuse layer model and augmented by a newly developed database of intrinsic constants for FeO<sub>3</sub> sorbents was tested on several saturated zone matrix materials. The algorithm successfully predicted sorption of several OSW metals, but failed for those metals that have predominantly anionic solution species (Cr, As, Se).

Draft final reports completed this quarter include:

- o Evaluation of the Application of Geochemical Equilibrium Programs to Regulatory Assessment.
- o A Pilot Study on the Selection of the Optimum Set of Components for Multicomponent Chemical Equilibrium Problems: Selection, Transformation, and Performance.

#### STATUS AND SCHEDULE OF DELIVERABLES:

- |      |   |            |
|------|---|------------|
| 8046 | DUE: 06/30/89    REVISED:   | COMPLETED: |
|      | Report on Impact of Treated Waste Forms on Exposure/Risk From Land Disposal of Hazardous Waste  |            |
|      | 8/87- added due to re-orientation of research program; this replaces #7353-A which was deleted since the contents of that project were no longer needed by the program office |            |
|      |   |            |
| 8159 | DUE: 07/31/89    REVISED:   | COMPLETED: |
|      | User's Manual for Site-Specific, Multimedia Model for Ranking Closure Options at RCRA Land Disposal Operations.   |            |
|      |   |            |
| 8160 | DUE: 08/31/90    REVISED:   | COMPLETED: |
|      | User's Manual for Model Defining Metal Species Transport in the Subsurface  |            |



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CODE TITLE

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

PPA (S): LAND DISPOSAL ASSESS

RC: K ERL ATHNS

PROJECT: 38 Environmental Process Characterization - Organics

PROJECT OFFICER: N. Lee Wolfe

PHONE: FTS-250-3429

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

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PROJECT DESCRIPTION:

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

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

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

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Studies of the effects of pH on the adsorption of anionic organic compounds to sediments have been initiated. Titration of a well characterized sediment using a pH-stat constructed here has shown that between the ambient pH value of 7.8 to approximately pH 5.5, hydrogen ion activity can be controlled by the addition of acid (HCl) to within about 0.5 units. Titration of pentachlorophenol (PCP, pKa equal to 4.8) between pH values of 7.8 and 4.0 in EPA 11 sediment (10 g sediment in 200 ml water) shows the concentration of pentachlorophenol in the aqueous phase to range from 80% of total added (at pH 7.8) to approximately 4% (at pH 4.0). Between pH values of 3 and 4, no difference was observed in the partition coefficient. This is highly consistent with octanol-water partitioning data for PCP in the same pH ranges. Further studies controlling the pH at higher values with the addition of base (NaOH)

are anticipated, along with titration of other compounds having different properties.

A draft paper on the homogeneous hydrolysis rate constants for selected chlorinated methanes, ethanes, ethenes and propanes has been written. This paper contains alkaline hydrolysis rate constants and activation parameters for 15 chlorinated hydrocarbons. The data will provide a basis for developing a structure reactivity relationship for estimation of rate constants for other halogenated hydrocarbons of importance to OSW. A draft journal article entitled "Hydrolysis of Chlorostilbene Oxide II. Hydrolysis in Aquifer Samples and in Sediment-Water Systems" contains results that provide support for a model that quantitatively describes abiotic hydrolysis in heterolytic systems.

A manuscript, "Reduction of Phorate Sulfoxide in Anaerobic Sediment Slurries," was submitted to Environmental Toxicology and Chemistry in November 1988. This paper describes hydrolysis and redox processes in sediment and soil samples. It shows that, at temperatures between 25 and 45 degrees C, reduction is the dominant transformation pathway, between 45 and 65 degrees oxidation dominates, and above 65 degrees hydrolysis dominates. A second paper, "Characterization of Reducing Properties of Anaerobic Sediment Slurries Using Redox Indicators," also submitted to Environmental Toxicology and Chemistry in November, provides a basis for using redox indicators as a tool to describe the redox state of sediments, soils and aquifer materials.

Kinetic studies of the degradation of Solvent Red 1 in anaerobic sediment-water systems show that the disappearance of the dye followed pseudo-first-order kinetics over two half-lives. The half-lives in two sediments were 94.6 and 67.9 hours.

Studies progressed on the degradation of diphenyl- and dialkyl-N-nitrosoamines in anaerobic sediments. While diphenyl-N-nitrosoamine was degraded to diphenylamine with a half-life of 11.8 hours, diethyl-, dipropyl-, and dibutyl-N-nitrosoamines were stable over a period of 14 days. Sorption studies indicate the dialkyl-N-nitrosoamines do not sorb to the sediment and that the diphenyl-N-nitrosoamine is only weakly sorbed. These results indicate that the dialkyl-N-nitrosoamines will be persistent and highly mobile in groundwater environments.

#### STATUS AND SCHEDULE OF DELIVERABLES:

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

12/86 - delay to 9/88 a result of G-R-H tap 3/86; 2/88 - delay to 7/89 a result of FY-88 Congressional Budget actions; 5/88 - transferred from D-109 D-54 during FY-89 PPA devel. process

7689 DUE: 12/30/88 REVISED: 04/30/89 COMPLETED:  
Report Describing the Kinetics of Redox Reactions in Soil-water  
Environments.

5/87 - due date revised during FY-88 PPA planning process as a result of reprogramming HW R&D resources into Wetlands program

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CODE TITLE

BUDGET SUB-ACTIVITY: D109 HAZARDOUS WASTE  
ISSUE: C WASTE CHARACTERIZATION  
PPA (L): 96 Waste Futures and Aquatic Impacts  
  
PPA (S): HW Aquatic Impacts  
RC: K ERL ATHNS  
PROJECT: 30 Assessment Methods for HW Characteristics and Constituents  
PROJECT OFFICER: Thomas Barnwell PHONE: FTS-250-3175

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

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PROJECT DESCRIPTION:

GOAL: Develop methods and models to predict (1) impact of future waste forms and regulatory levels on aquatic life and habitats and (2) regulatory thresholds for aquatic life and habitat impacts.

RATIONALE: OSW is redefining the waste characteristics that will set the future form, concentrations, and treatment levels for hazardous wastes. Little consideration has been given to aquatic impacts except as an exposure pathway to humans. Among these are organism toxicity, habitat alteration from oily wastes and sludges/slurries, and damages from flooded facilities. No methods exist to estimate the likelihood and consequences of future waste problems. Methods to properly define "safe" waste futures are not available for aquatic environmental impacts.

APPROACH: Relationships among future waste forms (component chemical concentration levels, treatment systems, oily wastes, disposal systems). release modes/rates and aquatic impacts will be identified and modeled within the OSW framework for defining appropriate waste characteristics. Data gaps will be identified and filled, and developed methodologies will be tested.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

This task is concerned with the development and validation of biological procedures that can be effectively used as part of monitoring efforts at hazardous waste sites. The procedure being evaluated is based on an ERL-Corvallis test for the bioassessment of waste site locations. The method has been tested at actual waste sites and found to be one of the better screening techniques for detecting the presence of potentially hazardous compounds. The current evaluation (and the subject of this quarterly report) will establish the data quality that can be achieved within a single laboratory, it will provide a basis for deciding whether the procedure merits collaborative testing and will more clearly define the method's potential for inclusion as part of an operational monitoring network.

The Chlorophyta Assay Using Soil and Sample Material is used to assess the potential toxicity of soil samples such as might be collected in the vicinity of hazardous waste sites. Water is added to individual soil samples and the resulting eluate is tested for toxicity using green algae (*Selenastrum capricornutum*). Since an aqueous eluate is initially acquired from the original

soil sample, and since this eluate is filtered and diluted prior to toxicity testing, the procedure does not really address nonwater soluble chemicals nor does it test for the presence of volatile compounds. In addition, problems associated with the collection of soil samples (e.g., representative sampling of a waste site area) are not addressed. Based on the ecological importance of unicellular algae, however, this relatively simple technique can provide an environmental hazard assessment for those chemicals that are, in fact, the compounds most likely to be transported to surface and ground waters.

The method protocol has been reviewed, revised, and reviewed a second time as steps toward achieving a "consensus" method. Water eluates were also taken from different types of soil, and tested using *Selenastrum* Sp., before a clay loam soil (characterized as being 22% sand, 51% silt, and 27% clay) was selected for use during the evaluation. After the soil selection was made, a suitable quantity of soil (approximately 275 kg) was collected so that enough soil would be available for the entire single laboratory effort. The soil was thoroughly homogenized, first by grinding, and then by being placed in a mechanical soil mixer and mixed for several hours. A ruggedness test, to identify procedural variables that must be carefully controlled, also was conducted.

If the Chlorophyta procedure is "rugged" it will not be susceptible to the inevitable, modest departures in routine and the final test result will not be altered by these slight variations. However, moderate procedural variations definitely altered the final Chlorophyta test result when they occurred at certain critical steps. Steps that must apparently be followed strictly as written concern the amount of water added to the dry soil sample, the pH of the resulting soil eluate that is actually used during the assay, and the specific eluate concentrations (dilutions) prepared for the assay dilution series. The Chlorophyta protocol has consequently been revised to emphasize strict adherence to these critical instructions.

The SARAH2 computational algorithms were completed this quarter. Work began on development of a new user interface using the AIDE user interface toolkit developed under the Ecorisk research program. This interface should be completed in early February 1989. Implementation of the Monte Carlo shell is on hold pending completion of the new interface.

A review of flooding regulations for solid waste management was completed by Aqua-Terra Consultants and delivered to Mark Schuknicht of OSW.

A report on feasibility of incorporation of the Habitat Suitability Index (HSI) in SARAH is under review by the authors (Aqua-Terra) and also will be complete by the end of January.

Significant technical support in support of hazardous waste characterization and aquatic impacts included:

- o Provided Bill Vocke, OSW Economic Analysis Branch, information on the oily waste model and CEAM work on wood-preserving waste for OSW and Superfund.

- o Sent Dr. Shih Chang, New Jersey Department of Environmental Protection, a set of chemical hydrolysis transformation rates, sorption coefficients, and water solubilities for use in landfill model in concentration based listing program.

#### STATUS AND SCHEDULE OF DELIVERABLES:

NO DELIVERABLES AVAILABLE

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CODE TITLE

BUDGET SUB-ACTIVITY: E104 PESTICIDES  
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION  
PPA (L): 07 GROUNDWATER: PEST. CONTAMINATION AND PROCESS STUDIES  
  
PPA (S): PEST. GROUNDWTR RES.  
RC: K ERL ATHNS  
PROJECT: 24 Validation of Predictive Techniques for Environ. Exposure  
PROJECT OFFICER: David S. Brown PHONE: FTS-250-3310  
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PLANNED START: 04/01/81 PLANNED END: 09/30/90  
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PROJECT DESCRIPTION:

GOAL: Refine, parameterize, and evaluate via field and other studies the capability of single and multimedia pesticide exposure models that predict the multimedia and intermedia transport and fate of pesticides, especially through soils (including an evaluation of their leaching potential), sediments, and other porous media to ground and surface waters.  
RATIONALE: Optimum pesticide regulation requires field-evaluated assessment techniques to assure that scientifically defensible decisions are made using cost-effective data specifications and assessment methods.  
APPROACH: As single and multimedia pesticide exposure assessment packages are developed or assembled from SOA components on application/drift, runoff, leaching, surface stream, river and lake simulation, etc., and become operational, they will be systematically evaluated via application to "real world" OPP and state problems and via retrospective comparison studies. Limited special field studies also will be initiated in concert with OPP, states, Regions, and other agencies to generate required data bases to test either complete model packages or specific components. Current emphasis is on the Dougherty Plain leaching study.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

All monitoring equipment was removed from the Dougherty Plain test site and the site was released to the cooperating farmer. An additional set of 597 soil samples were taken for bromide tracer analysis from sidewalls, the large excavations developed in removing monitoring test equipment. Analysis of both soil and water samples for bromide tracer continued during the quarter. A total of 3700 bromide samples have been analyzed to date for use in testing and calibrating the pesticide transport codes PRZM/RUSTIC.

A manuscript entitled "A Method for Testing Whether Model Predictions Fall within a Prescribed Factor of True Values with Application to Pesticide

Leaching", was completed during the quarter and submitted to Water Resources Research. This work describes a quantitative method for evaluating model performance at the field level and is viewed as a significant new contribution in the field of model testing. Generally, the technique should be applicable to a variety of environmental pollutant transport and transformation models.

Plans were developed for a multiagency cooperative field research project on pesticide leaching at a new field site near Plains, GA. Three agencies--EPA, USDA and USGS--will cooperate at the site in an effort to maximize efficiency and reduce costs of model testing.

Mr. Charles Smith was appointed as the laboratory representative for the Environmental Monitoring and Assessment (EMAP) Project Agroecosystem Work Group and attended the planning workshop held in Chicago, October 24-27, 1988. Substantial follow-up planning activities also have taken place during the quarter.

#### STATUS AND SCHEDULE OF DELIVERABLES:

7661 DUE: 09/30/89 REVISED: COMPLETED:  
Final Dougherty Plain Report Including Pesticide Ground Water Threat  
Assessment Method

5/88- title change during FY-89 PPA devel.

7664 DUE: 06/30/89 REVISED: COMPLETED:  
Project Report on Soils Data Based for RUSTIC Model (Linked PRZM-Groundwater  
Model)

5/88 - title change

8196 DUE: 12/31/90 REVISED: COMPLETED:  
Report on Testing RUSTIC Model Using Selected Data Bases

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

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

PPA (S): DEVELOP PRED. TECH.

RC: K ERL ATHNS

PROJECT: 14 Pesticide Process Characterzation

PROJECT OFFICER: Arthur W. Garrison PHONE: FTS-250-3145

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

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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 (ionizable) pesticides to soils and sediments will be emphasized.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Studies of the effects of pH on the adsorption of anionic organic compounds to sediments have been initiated. Titration of a well characterized sediment using a pH-stat constructed here has shown that, between the ambient pH value of 7.8 to approximately pH 5.5, hydrogen ion activity can be controlled by the addition of acid (HCl) to within about 0.5 units. Titration of pentachlorophenol (PCP, pKa equal to 4.8) between pH values of 7.8 and 4.0 in EPA 11 sediment (10g sediment to 200ml water) shows the concentration of pentachlorophenol in the aqueous phase to range from 80% of total added (at pH 7.8) to approximately 4% (at pH 4.0). Between pH values of 3 and 4, no difference was



observed in the partition data for PCP in the same pH ranges. Further studies controlling the pH at higher values with the addition of base (NaOH) are anticipated, along with titration of other compounds having different properties. Aqueous phase metals have been measured by ICP to assess the effects of the pH changes on the dissolution and precipitation of inorganic species and their possible relationship to organic anion partitioning.

A manuscript, "Reduction of Phorate Sulfoxide in Anaerobic Sediment Slurries," was submitted to Environmental Toxicology & Chemistry in November 1988. This paper describes hydrolysis and redox processes in sediment and soil samples. It shows that at temperatures between 25 to 45 degrees C reduction is the dominant transformation pathway, between 45 and 65 degrees C oxidation dominates, while above 65 degrees C hydrolysis dominates.

A second paper, "Characterization of Reducing Properties of Anaerobic Sediment Slurries Using Redox Indicators," also submitted to Environmental Toxicology & Chemistry in November, provides a basis for using redox indicators as a tool to describe the redox state of sediments, soils and aquifer materials.

STATUS AND SCHEDULE OF DELIVERABLES:

8197 DUE: 06/30/90 REVISED: COMPLETED:  
Report on Sorption of Water Soluble Ionic Pesticides to Soils and Sediments.

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

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

PPA (S): DEVELOP PRED. TECH.

RC: K ERL ATHNS

PROJECT: 25 Predictive Techniques for Environmental Exposure

PROJECT OFFICER: David S. Brown PHONE: FTS-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 OTS and OW are envisioned and required, e.g. PMN assessments.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Efforts during the quarter focused on completion and documentation of the code linkages required in assembling the new linked root zone, vadose zone, saturated zone pesticide transport model RUSTIC. A work assignment for additional testing of the linked code and beta testing versions was distributed to three cooperators. So far some differences have been found in the VAX and Prime versions and these problems are undergoing further investigation.

A series of 40 Pesticide Root Zone Model (PRZM) input scenarios were developed and provided to CAD West for the Sun Computer Development Project.

Ongoing technical assistance efforts to the PRZM Users Group continued

during the quarter. A variety of technical, scientific, and computer-related questions were handled by phone.

Technical assistance was provided to OPP, as requested by Catherine Eiden, concerning technical approaches to modeling behavior of pesticides used in ship paints in the New York, San Diego Bay and Norfolk harbors.

Review, evaluation and testing of the overlay structure for PC implementation of RUSTIC is underway.

STATUS AND SCHEDULE OF DELIVERABLES:

NO DELIVERABLES AVAILABLE

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

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

PPA (S): INTEGRATED RISK ASS.

RC: K ERL ATHNS

PROJECT: 26 Risk Assessment Methods for FIFRA

PROJECT OFFICER: David S. Brown

PHONE: FTS-250-3310

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

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PROJECT DESCRIPTION:

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

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

APPROACH: Existing unsaturated/saturated zone soil transport models, proven runoff-surface water pesticide codes, appropriate ground water codes, and related air transport models will be combined to produce SOA exposure assessment model frameworks. 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, RSKERL, AREAL and the aquatic fate research at AERL.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Mr. Jeff Scarbrough is developing a ground spray application module for the new Terrestrial Ecosystem Exposure Assessment Model (TEEAM) and has been working to eliminate some minor "bugs" discovered in the present aerial spray application code.

Mr. Mark Cheplick carried out further development and testing of TEEAM during the quarter and has begun a series of sensitivity tests initiated in the hope of finding appropriate ways to streamline the code.

A draft report outlining results of initial TEEAM sensitivity tests was

completed is under review. The report is entitled "Sensitivity Analysis of the Terrestrial Ecosystem Exposure Assessment Model."

STATUS AND SCHEDULE OF DELIVERABLES:

- 8129 DUE: 02/28/89 REVISED: COMPLETED:  
Users Manual and User Interface Toolkit for Exposure Assessment Models
- 8130 DUE: 08/31/89 REVISED: COMPLETED:  
Report: Sensitivity Analyses and Preliminary Testing of the Terrestrial  
Ecosystem Exposure Assessment Model
- 8131 DUE: 08/31/90 REVISED: COMPLETED:  
Users Manual for Updated TEEAM Model

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXICS  
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION  
PPA (L): 09 DEVELOPMENT OF VALIDATED EXPOSURE ASSESSMENT METHODOLOGIES  
  
PPA (S): EXPOSURE ASSESSMENT  
RC: K ERL ATHNS  
PROJECT: 12 Development of EcoRisk Exposure Models  
PROJECT OFFICER: Craig Barber PHONE: FTS-250-3147  
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PLANNED START: 10/01/87 PLANNED END: 12/31/99  
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PROJECT DESCRIPTION:

GOAL: 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 that can use readily available chemical parameters to make predictions.  
APPROACH: Exchange models will be developed to provide estimates of body burdens of representative chemicals. Models will be based on thermodynamic principles and morphometric characteristics of organisms as well as on consideration of 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 entitled "Modeling Bioaccumulation of Organic Pollutants in Fish with an Application to PCBs in Great Lake Salmonids" was submitted to the Canadian Journal of Fisheries and Aquatic Sciences.

Work was begun to extend FGETS' capabilities so that bioaccumulation of ionizable organic chemicals can be simulated. Because, in the absence of specific transport mechanisms, only the neutral species of an ionizable chemical is exchanged across biological membranes, it was initially thought that this extension to FGETS would simply require computational algorithms to estimate the water concentrations of the exchangeable species. A compilation of

a small data set of published studies on the bioaccumulation of various chlorophenols indicated that this logic was incorrect because uptake rates predicated by FGETS adjusted for effective concentration were one or two orders of magnitude lower than observed values. Such underestimation could result either because the ionized species is also exchanged or because the transport conductance of the neutral species of an ionizable chemical through the interlamellar water of a fish's gills is enhanced by the chemical's dissociation reaction. The latter explanation is currently being investigated by constructing analytic solutions to the partial differential equations that describe mass diffusion with forced convection in flat channels under boundary conditions that are thought to emulate those associated with ionizable chemicals.

Early in December, Dr. David Randall and Dr. Larry Fiddler visited ERL-Athens to discuss how their studies in fish respiratory physiology might interface or help support our bioaccumulation modeling. It was clear that their work on ammonia and carbon dioxide exchange across fish gills was of immediate importance to our current work involving ionizable chemical because carbon dioxide excretion alters the pH and hence the concentration of the neutral species of an ionizable chemical in the interlamellar water of the gill. It would be desirable and advantageous to foster this continued interaction if R&D resources are available.

#### STATUS AND SCHEDULE OF DELIVERABLES:

8135	DUE: 02/28/89	REVISED:	COMPLETED:
	Research Brief: Modeling bioaccumulation of polar and ionic chemicals by fish.		

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE  
BUDGET SUB-ACTIVITY: L104 TOXICS  
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION  
PPA (L): 09 DEVELOPMENT OF VALIDATED EXPOSURE ASSESSMENT METHODOLOGIES  
PPA (S): EXPOSURE ASSESSMENT  
RC: K ERL ATHNS  
PROJECT: 27 Development of Validated Exposure Assessment Methodologies  
PROJECT OFFICER: Thomas Barnwell PHONE: FTS-250-3210  
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PLANNED START: 10/01/79 PLANNED END: 12/31/99  
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PROJECT DESCRIPTION:

GOAL: Develop, parameterize and evaluate multimedia modeling systems and continue development and modification of existing models for non-human exposures.

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

APPROACH: Thermodynamic metal species and chemical reaction models will be combined with partitioning and bioaccumulation (including plants) models to produce a process-based aquatic distribution package for metal species. 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:

A standard Fortran-77 computer code of the preliminary 3-D estuary and lake sediment transport model was completed. The initial code also was documented. This initial code will be tested at AREAL in the second quarter and will be implemented for the Green Bay application. To aid early testing, 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 additional development of the sediment dispersion model and testing with Lake Okeechobee data. Processing of the initial data is continuing.

ASCI tested and debugged the hydrodynamics code delivered last quarter. A preliminary test data set for Green Bay was compiled and the code was put on



a faster computer. A bathymetry data set and segmentation scheme was devised as well as a wind field processor and tidal boundary option.

In the second quarter the preliminary sediment transport code will be tested followed by testing and documentation of the hydrodynamics code. A preliminary data set for the Green Bay Application of the Sediment Transport Model will be developed and additional assistance will be provided to other Green Bay researchers by defining the general hydrodynamics and required linkage to the WASP model.

STATUS AND SCHEDULE OF DELIVERABLES:

8047 DUE: 08/31/89 REVISED: COMPLETED:  
Final Report on Monte Carlo Version of MINTEQ

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS

Office of Environmental Processes and Effects Research

ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXICS  
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION  
PPA (L): 10 TRANSPORT AND FATE PROCESS DETERMINATION

PPA (S): TRANSPORT AND FATE

RC: K ERL ATHNS

PROJECT: 09 Chemical Process Characterization for Toxics

PROJECT OFFICER: Richard G. Zepp PHONE: FTS-250-3428

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

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PROJECT DESCRIPTION:

GOAL: Characterize key chemical processes (direct-indirect photolysis, hydrolysis, redox reactions, and sorption/desorption) and expand scientific understanding of sediment-water exchange to improve exposure and risk assessment models for PMN chemicals.

RATIONALE: The role 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; for example, some dyes are rapidly degraded in sediment-water systems.

APPROACH: Laboratory studies using natural waters, sediments and reference materials will be used to accept or reject proposed equations for the kinetics and equilibria of transformation and sorption processes. Rate and equilibrium constants to fit the equations will be provided. Compounds and reaction conditions will be selected to permit generalizations about changes in molecular structure and environmental composition. Photochemical studies will emphasize the role of naturally occurring inorganic species; redox reactions of abiotic systems, relative to biotic systems, will be studied. Chemical fate processes of azo and anthroquinone dyes will receive particular attention.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A draft paper on the homogeneous hydrolysis rate constants for selected chlorinated methanes, ethanes, ethenes and propanes has been written. This paper contains alkaline hydrolysis rate constants and activation parameters for 15 chlorinated hydrocarbons. The data will provide a basis for developing a structure reactivity relationship for estimation of rate constants for other halogenated hydrocarbons. A draft journal article entitled "Hydrolysis of Chlorostilbene Oxide II. Hydrolysis in Aquifer Samples and in Sediment-Water Systems" contains results that provide support for a model that quantitatively describes abiotic hydrolysis in heterolytic systems.

Kinetic studies of the degradation of Solvent Red 1 in anaerobic sediment-water systems show that the disappearance of the dye followed pseudo-first-order kinetics over two half-lives. The half-lives in two sediments were 94.6 and 67.9 hours.

Studies progressed on the degradation of diphenyl- and dialkyl-N-nitrosoamines in anaerobic sediments. While diphenyl-N-nitrosoamine was degraded to diphenyl-amine with a half-life of 11.8 hours, diethyl-, dipropyl-, and dibutyl-N-nitrosoamines were stable over a period of 14 days. Sorption studies indicate the dialkyl-N-nitrosoamines do not sorb to the sediment and that the diphenyl-N-nitrosoamine is only weakly sorbed. These results indicate that the diphenyl-N-nitrosoamines will be persistent and highly mobile in groundwater environments.

Studies of the effects of pH on the adsorption of anionic organic compounds to sediments have been initiated. Titration of a well characterized sediment using a pH-stat constructed here has shown that, between the ambient pH value of 7.8 to approximately pH 5.5, hydrogen ion activity can be controlled by the addition of acid (HCl) to within about 0.5 units. Titration of pentachlorophenol (PCP, pKa equal to 4.8) between pH values of 7.8 and 4.0 in EPA 11 sediment (10 g sediment in 200 ml water) shows the concentration of pentachlorophenol in the aqueous phase to range from 80% of total added (at pH 7.8) to approximately 4% (at pH 4.0). Between pH values of 3 and 4, no difference was observed in the partition coefficient. This is highly consistent with octanol-water partitioning data for PCP in the same pH ranges. Further studies controlling the pH at higher values with the addition of base (NaOH) are anticipated, along with titration of other compounds having different properties.

Research was continued on the influence of light on the oxidation of organic substrates by manganese oxides. Kinetic studies of the oxidation of p-chlorophenol were conducted using monochromatic radiation corresponding to the maximum absorption of manganese dioxide (336 nm). The pH dependence of the oxidation rate of p-phenylphenol in manganese oxide suspensions exposed to sunlight also was investigated. Studies of the influence of light on the oxidation of anilines by manganese oxides were initiated; the oxidation of p-chloroaniline was examined. Work on the photoredox reactions of copper were also continued. Quantum yields were determined as a function of pH for the photoreduction of copper (II) complexed by nitrogen ligands. Kinetic studies were conducted in sunlight for comparison. Two journal articles were submitted for publication during the quarter: "Hydrogen Peroxide Decay in Waters with Suspended Sediments: Evidence for Biologically Mediated Processes" and "Aquatic Humic Substances as Sources and Sinks of Photochemically Produced Transient Reactants."

#### STATUS AND SCHEDULE OF DELIVERABLES:

8137 DUE: 03/30/90 REVISED: COMPLETED:  
Internal Report - (Research Brief) - Fate of Dyes in the Environment.

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXICS  
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION  
PPA (L): 10 TRANSPORT AND FATE PROCESS DETERMINATION

PPA (S): TRANSPORT AND FATE

RC: K ERL ATHNS

PROJECT: 37 Microbial Transformation Rate Constants

PROJECT OFFICER: William C. Steen

PHONE: FTS-250-3776

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

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PROJECT DESCRIPTION:

GOAL: Develop and apply a system that provides, on a timely basis, second order microbial transformation rate constants for suspended organisms in aerobic aquatic systems.

RATIONALE: Under the Toxic Substances Control Act, both new and existing chemicals must be evaluated for potential to pose environmental risk from the standpoint of toxicity. A major consideration in assessing environmental exposure is microbial transformation. Second order rate constants provide a means of evaluating potential for microbial transformation at various environmental microbial population levels.

APPROACH: Reproducible second order rate constant measurement techniques will be established to relate all chemicals to the same population conditions. Second order microbial transformation rate constants will be measured for selected chemicals representing each important class of chemicals. Relationships between microbial transformation rate and molecular spectroscopic properties will be established for base compounds in each chemical class. Rate constants for additional compounds of interest will be inferred from their molecular spectroscopic properties, which are easily measured.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Second order microbial transformation rate constants were completed for seven substituted amides for use as PNN analogies. They are tabulated below:

k(b) = L per org. per hr.

Propachlor	1.1 X E-9
Proporial	5.0 X E-10
N-methylbenzamide	1.0 X E-12
Monalide	6.0 X E-13
Alachlor	3.0 X E-13

Pronamide	5.0 X E-14
Niclosamide	2.0 X E-14

Measurements were made using the ERL-Athens protocol for suspended organisms in aerobic systems.

Compilation has begun on vibrational spectra in different media for the substituted amides. These data will be used in conjunction with microbial degradation data both to extend property-reactivity correlations (PRCs) and to develop some understanding of the importance of solvent effects.

A new approach to PRCs is being investigated that offers the promise of utilizing more of the available spectral information than is used at present in arriving at correlations. Because more independent data are used, correlations should be more reliable.

In conjunction with the PRCs of biolysis rate constants and spectroscopic properties mentioned last month, preliminary work is in progress to test the feasibility of direct aqueous injection GC/FT-IR as an alternative to LC/FT-IR. LC/FT-IR is a much more difficult technique to use, but is generally considered to be essential for those compounds that are not amenable to simple extraction into a non-polar medium. Successful direct aqueous injection GC/FT-IR will simplify the identification of low-level, water-soluble compounds both for the PRC work and for multi-spectral identifications.

Second order rate constants were measured for acetanilide ( $1.4 \times 10^{-11}$ ) and benzanilide ( $2.4 \times 10^{-12}$ ). These data and the rate constants reported for six compounds last quarter will be compared with spectroscopic properties to assess PRCs.

Four substituted sulfonyl urea herbicides were selected for measurement of second order microbial rate constants for PRCs.

#### STATUS AND SCHEDULE OF DELIVERABLES:

8136 DUE: 08/31/90 REVISED: COMPLETED:  
Report: Microbial Transformation Rate Constants of Structurally Diverse  
Man-made Chemicals.

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXICS  
ISSUE: D ECOLOGY: TRANSPORT/FATE/FIELD VALIDATION  
PPA (L): 11 EVALUATION OF EXPOSURE ASSESSMENT METHODS  
  
PPA (S): MICROCOSM/FIELD  
RC: K ERL ATHNS  
PROJECT: 05 Environmental Transformation and Equilibrium Constants  
PROJECT OFFICER: Heinz Kollig PHONE: FTS-250-3770  
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PLANNED START: 10/01/83 PLANNED END: 12/31/99  
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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 computerized Coordinated List of Chemicals (CLC) database, which tells who is studying what chemical in ORD, was compiled into a computer executable form. The database can now be used on a PC without any additional software.

A prototype computerized quality evaluation system for the water solubility of pesticides, developed by the Agricultural Research Service, USDA, was reviewed. The system should be useful in evaluating water solubility data for any organic chemical.

Work continued on the development of the fate constant database with FOCUS.

STATUS AND SCHEDULE OF DELIVERABLES:

7905 DUE: 03/31/89 REVISED: COMPLETED:  
Report on problems associated with published environmental fate constants

5/88 - title change



PRINT DATE: 01/30/89  
PMS-060

CLIENT OFFICE OTS

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
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ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

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

PPA (S): MICROCOSM/FIELD

RC: K ERL ATHNS

PROJECT: 16 Evaluation of Exposure Assessment Methods

PROJECT OFFICER: David L. Lewis

PHONE: FTS-250-3358

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

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PROJECT DESCRIPTION:

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

RATIONALE: Methodologies for predicting and/or assessing ecological 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:

A completed model of the entire surface water system of the Netherlands was received. Analysis of the model revealed a number of features that will require correction. Simulation studies of four test chemicals demonstrated that most of the segments are advection dominated and thus of relatively slight value in testing process models. The Dutch Laboratory RIVM is assembling a more detailed dataset that is less advection dominated for process model testing. Additional chemicals for process model testing will be identified in the coming quarter via analysis of the Dutch WAKWAL monitoring system.

Inhouse laboratory experiments to test the hypothesis of a threshold critical aqueous blood concentration of a toxicant at which effects on an organism occur are continuing using the neutral hydrophobic test chemical 1,2,3,4-tetrachlorobenzene (TCB). These studies are needed to test FGETS and



for development of effects models and are not being done anywhere else. Because of wide ranges in results for plasma and whole body concentrations of TCB and plasma content of lipid and moisture, a large amount of effort this quarter has been on quality assurance for all these analyses. We are now confident the simplified extraction method being used is as efficient and consistent as the approved sonication method used by Region IV for extraction of organics. Therefore, the variation in the TCB data is real. Plasma lipid and moisture determinations have been modified and refined, and we now have confidence in those parameters.

The hard-to-define endpoints with the narcotic chemical, TCB, are still a problem. Bluegill sunfish exposed then sampled when near death or dead (24 to 48 hrs) have plasma TCB concentrations of from 128 to 775 mg/kg, whereas individuals removed at turnover (1 to 2 hrs) have plasma TCB concentrations within the same range. At this point the hypothesis of a lethal threshold in the blood for TCB does not seem realistic. Whole body concentrations of TCB, however, do show some correlation with death and both parameters are being further studied.

Ongoing and future studies include sequential sampling of blood from a living channel catfish during exposure to TCB to determine uptake into the blood with time; exposure and sampling of more bluegills to obtain more complete datasets; and exposure of guppies to compare whole body concentrations at death with those in a study in the literature by van Hoogen and Opperhuizen. The project is behind schedule because of very time consuming and specific analyses, and the large amount of quality assurance work required. New target date is March 1989.

A report on an Exposure Analysis Modeling System (EXAMS) subroutine for predicting microbial transformation rates by biofilms (Gattie, Lewis, Newton) has been written and is being internally reviewed.

#### STATUS AND SCHEDULE OF DELIVERABLES:

8138 DUE: 07/31/89 REVISED: COMPLETED:  
Report: EXAMS subroutines for predicting microbial transformation rates of aquatic pollutants by attached populations.

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXICS  
ISSUE: G STRUCTURE ACTIVITY RELATIONSHIPS  
PPA (L): 20 STRUCTURE-ACTIVITY RELATIONSHIPS AND ESTIMATION TECHNIQUES  
PPA (S): SAR/EST TECHNIQUES  
RC: K ERL ATHNS  
PROJECT: 10 Predictive Methods for Environmental Exposure Assessments  
PROJECT OFFICER: Samuel W. Karickhoff PHONE: FTS-250-3149

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

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PROJECT DESCRIPTION:

GOAL: Develop and test concepts for predicting key environmental transport and transformation processes for exposure and risk assessments of PMN chemicals.  
RATIONALE: Computational procedures are needed for estimation of photochemical, hydrolytic and other transformation rate coefficients 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 transformations and for acidity constants (pKa). Process rate and equilibrium constants then will 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:

The pKa's of esters are being catalogued for continued testing of SPARC, the ERL-Athens expert system for predicting chemical reactivity parameters such as pKa, hydrolysis rate constants, UV absorption spectra (for photochemical degradation rate constants), etc. Rearrangement of Prolog code for SPARC into stand-alone modules has begun, as well as documentation of Prolog code. Development of an interface for the spectra database (currently for 200 compounds) with SPARC is still in progress.

Three journal articles describing SPARC and its preliminary applications are now being cleared at ERL-Athens for publication in one issue of Environmental Toxicology and Chemistry.

STATUS AND SCHEDULE OF DELIVERABLES:

8144 DUE: 08/31/90 REVISED: COMPLETED:  
Report documenting application of expert systems for predicting reactivity parameters for PMN chemicals



PRINT DATE: 01/30/89  
PMS-060

CLIENT OFFICE OTS

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS

Office of Environmental Processes and Effects Research

ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

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

PPA (S): SAR/EST TECHNIQUES

RC: K ERL ATHNS

PROJECT: 15 PRC Relationships and Other Estimation Techniques

PROJECT OFFICER: Susan A. Moore

PHONE: FTS-250-3469

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

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PROJECT DESCRIPTION:

GOAL: Expand data bases for establishing property reactivity correlations (PRC) and develop quantitative relationships between microbial rate constants and molecular descriptors.

RATIONALE: There is a need for developing predictive models for fate and effects based on structure activity relationships /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 toxic chemicals. Emphasis will be placed on measurements of biomass associated with transformations. A homologous series of compounds will be used to examine how 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:

Changes in river water that occur when it is stored for extended periods in the laboratory were investigated. The significance is, first, that the degradative activity of river water may change during storage leading to inaccurate conclusions about the degradative activity of the natural setting. The goal, therefore, is to identify conditions in which river water can be stored in a pristine state. Second, changes in river water that are induced by varying the storage conditions are likely to mimic or approximate natural changes due to seasonal and environmental factors, hence identifying such factors. A second river water sample was collected and previous results were confirmed and extended. Storage conditions have not yet been found that maintain river water in its original state, but progress has been made. Storage of 20 degrees Centigrade river water at 20 degrees Centigrade for 40 days produced no significant change in total cell concentration, but the frequency of occurrence of cell strains changed markedly (based on visual

inspection of agar plates). In contrast, storage at -72 degrees Centigrade produced a 20-fold decrease in cell concentration after 3 days although the frequency of cell strains appeared to remain constant up to 40 days. Storage at 3 and -12 degrees Centigrade produced results that were intermediate between those at 20 and -72 degrees Centigrade. A microplate assay was initiated to identify cell strains in river water and better quantitate their frequencies of occurrence. Cell concentration was measured as both CFU on agar plates and MPN in liquid medium. Controls ruled out so called "bottle effects" and effects due to the thickness of agar on agar plates. Rapid freezing and storage in liquid nitrogen (approximately -200 degrees C) is being tested. It may be that river water must be reconstituted from stored components in order to (re)obtain the original state and allow accurate, reproducible laboratory analysis of biodegradation. The doubling times in rich medium of the fastest growing cells that were endogenous to river water were measured in a spectrophotometric assay. Between 10 and 30 degrees Centigrade, a 10-fold increase in temperature produced a 2.2-fold increase in cell growth rate. Theoretical analysis of biodegradation by Michaelis-Menten and Monod kinetics was continued with a view towards distinguishing between them. Monod kinetics are likely to represent complete degradation of xenobiotics to CO<sub>2</sub> in contrast to the buildup of side products that is typical of Michaelis-Menten kinetics. Analysis of physical properties was continued on a second sample of river water. Ultrafiltration was used to separate components by molecular weight, and methods for routine organic carbon analysis were initiated. Degradation studies were begun. Three out of ten samples randomly picked but visually distinct clones of microbes from river water were found to degrade 4-chloro-aniline within 10 days after inoculation in basal salts medium.

#### STATUS AND SCHEDULE OF DELIVERABLES:

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

5/88- title and due date changed during FY-89 PPA devel.

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXICS  
ISSUE: I ECOLOGY: ECTOXICITY AND RISK ASSESSMENT  
PPA (L): 26 DEVELOP METHODOLOGIES FOR ECOLOGICAL RISK ASSESSMENT

PPA (S): RISK ASSESSMENT DEV.

RC: K ERL ATHNS

PROJECT: 13 Predictive Techniques for Ecological Risk

PROJECT OFFICER: Ray R. Lassiter

PHONE: FTS-250-3208

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

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PROJECT DESCRIPTION:

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

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

APPROACH: Exposure analysis models will be used to provide expected aquatic environmental concentration distributions. To develop the capability to analyze for expected effects, it will be necessary, first, to determine what effects are of concern (population, community, second, ecosystem), and the appropriate aquatic systems to use to study those effects, and second, 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:

Recruitment was completed for a microbiologist/modeler this quarter. Selected candidate is Dr. Rochelle Aurajo from Cornell University, who will report to the project on April 9, 1989.

Work continued this quarter in design of an experimental GIS interface between biological distribution data and simulation model parameter sets. Accounts for all project personnel were established on the NCC VAX, and authorizations were obtained for use of VAX ARC/INFO on the CASTOR (VAXB) node. The Tektronix 4106 terminal and Tektronix 4105 emulation using PCPLOT+ on the PC workstations were set up and tested using VAX sample datasets. Integration of PC ARC/INFO and the NCC VAX version was tested using a sample Digital Line Graph (DLG) provided by the United States Geological Survey (USGS) on magnetic tape for the Chattanooga area. A Bailey ecoregion coverage was designed, and a

crop capability class mapping from USDA/ARS was located for possible use. These coverages will be implemented in the second quarter of FY89. The availability of digital data for potential study sites in Georgia, Alabama, and Louisiana was evaluated as part of general study design and feasibility exercises.

Steps for planning the 1989 Ecorisk All Investigators Meeting have been taken. Tentatively the meeting will be held in Athens during the last week of February. Contact persons at the other Ecorisk laboratories will be contacted during the first 2 weeks of January to finalize the necessary arrangements.

In December ERL-Athens principals met to evaluate the status and direction of the Ecorisk Research Program with respect to the integration of existing Ecorisk databases and models into Ecorisk Assessment tools that can be used by OTS. Although no definitive decisions were made, several important topics were addressed. These include: (1) Should the research of the Ecorisk program be incorporated into a series of assessment softwares or into a single system like GEMS? (2) Is there duplication of effort in the Ecorisk program, for example, (a) FGETS and the Erickson/McKim gill model, (b) the ERL-Athens/UGA physiological/ecological database and the Dutch biological database, and (c) the Biology Branch's planned EXAMS/FGETS/FIS software system and the existing CADSWES Sun-based system supported by the Assessment Branch? (3) Should the integration of existing Ecorisk databases and models be emphasized during the 1989 All Investigators's meeting?

Habitat associations for approximately 40 species (aquatic and terrestrial) selected from the USFWS Endangered and Threatened Wildlife and Plants List are still being acquired. Data have come from USFWS publications, the Endangered Species Information System (ESIS), and the Multi-State Fish and Wildlife Information System. The BIOTA database will be linked to several data layers (land use/land cover, hydrography, political boundaries, etc.) currently under development for a GIS-based management tool to determine species-at-risk and parameterize exposure and effects models.

The cooperative agreement with Montana State University and the University of British Columbia is showing good progress. This work is in support of the Ecorisk modeling efforts. Most of the preliminary studies on the respirometer itself, introduction of chemicals and their behavior in the respirometer, determination of the most significant tissues to analyze, and analysis of 1,2,3,4-tetrachlorobenzene (TCB) uptake by rainbow trout have been performed both under static conditions and in the respirometer under different water velocities or forced swimming speeds. Uptake of TCB into various tissues (plasma, adipose, pink muscle, white muscle, liver, brain, heart, kidney, liver, gut, upper gut, gills, and spleen) has been determined in fish sacrificed times up to 6 hours. The results indicate that the body burden of the toxicant increased and oxygen uptake increased with swimming speed. Also tissue levels of the toxicant showed a constant ratio to the plasma level independent of both swimming speed and time of exposure.

The competitive cooperative agreement on prediction of the effects of toxicants on natural aquatic populations and biological communities is proceeding on schedule. Three preproposals were received and are currently in the review process.

Ms. Sue Wolf presented the paper "Neutral chemical accumulation in aquatic

plant shoots" at the Ninth Annual Meeting of the Society of Environmental Toxicology and Chemistry (SETAC). Dr. Ray Lassiter and Steven Wooten coauthored the paper. Ms. Wolf was invited by Dr. D. MacKay to present the paper at the workshop "Human exposure to chemicals" held at the Institute for Environmental Studies (University of Toronto, Canada). Both presentations were well received.

STATUS AND SCHEDULE OF DELIVERABLES:

7510 DUE: 08/31/88 REVISED: 08/31/90 COMPLETED:  
POPULATION MODEL AND SOFTWARE INCORPORATING LETHAL AND NONLETHAL EFFECTS  
ON FEEDING BEHAVIOR FOR CHEMICALS THAT ACT BY REVERSIBLE MODES OF ACTION

2/87- due date revised per Russo memo 2/6/87; 5/87 - due  
date revised to 8/90 during FY-88 PPA planning process as a  
result of reductions in planned resources

7512 DUE: 08/31/88 REVISED: 08/31/90 COMPLETED:  
DOCUMENTATION REPORT ON SPECIFICATIONS FOR INPUT PARAMETERS AND COMPUTER  
CODE FOR AQUATIC ECOSYSTEM MODELS

5/87 - due date revised to 8/90 during FY-88 PPA planning  
process as a result of reductions in planned resources

7513 DUE: 08/31/90 REVISED: 08/31/92 COMPLETED:  
COMPUTER CODE FOR FIRST OPERATIONAL VERSION OF AN ECOLOGICAL EFFECTS MODEL  
FOR AQUATIC ECOSYSTEMS

5/87 - due date revised to 8/92 during FY-88 PPA planning  
process as a result of reductions to planned resources

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

5/87 - due date revised to 8/93 during FY-88 PPA planning  
process as a result of reductions in planned resources

8146 DUE: 05/31/89 REVISED: COMPLETED:  
Internal Report: Products of the Ecorisk Research Program.





FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXICS  
ISSUE: I ECOLOGY: ECTOXICITY AND RISK ASSESSMENT  
PPA (L): 26 DEVELOP METHODOLOGIES FOR ECOLOGICAL RISK ASSESSMENT

PPA (S): RISK ASSESSMENT DEV.

RC: K ERL ATHNS

PROJECT: 28 Risk Assessment Methodologies for Toxic Substances

PROJECT OFFICER: Tom Barnwell PHONE: FTS-250-3160

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

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PROJECT DESCRIPTION:

GOAL: Develop computerized risk assessment systems that help 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 costs.

APPROACH: Existing software will be reviewed including GEMS, ANNIE, and the IIASA-IRIMS system. Related 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 in laboratory and field studies to optimize risk assessment procedures.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

PC-GEMS distribution and full-fledged use began this quarter by the Office of Toxic Substances, in cooperation with the University of Wisconsin Continuing Education Program, which began advertising a short course on PC-GEMS.

Dr. Steve Chapra and Mr. Jim Waterman of the University of Colorado visited ERL-Athens to present a seminar on progress to date and to discuss further work. They obtained a copy of the PRZM model to design a new graphics interface. The PRZM graphics interface will be implemented on a DEC MicroVAX GPS workstation in order to insure compatibility with ORD hardware.

The ANNIE-EMIFE integration is proceeding smoothly. A draft report was received this quarter and both manual and software were reviewed in depth. Comments were received from reviewers at the USGS and from inhouse CSC programmers. The software is currently being used inhouse to develop an interface for the SARAH model. A short course to teach inhouse staff and other interested personnel use of the software is tentatively planned for April.

A short course on Exposure and Bioaccumulation Models is tentatively planned for Athens the week of July 24-28. The course will be similar to the two courses presented in Washington DC and Boulder CO last summer.

Dr. James Hill has prepared a paper, "Error Analysis of Two Aquatic Bioaccumulation Models," that will be submitted to a journal in the second quarter. The paper compares the Thomann-Connolly bioconcentration model to the EPA Food and Gill Exchange of Toxicants (FGETS) model.

#### STATUS AND SCHEDULE OF DELIVERABLES:

7497 DUE: 09/30/88 REVISED: 11/30/89 COMPLETED:  
Users Manual for Update Stratified Lake Transport Model for Risk Assessment

to 9/89 as a result of P.O. receiving an OEPER FY-87 2% Set Aside Award for a research project; 6/88 - title change and due date to 11/89 due to delay in hiring qualified modeler contractor

7499 DUE: 09/30/88 REVISED: 08/31/90 COMPLETED:  
General Bed-Water Exchange Model for Risk Assessment

2/87- due date revised to 9/89 per Russo memo 2/6/87; 6/88 due date to 8/90 due to ecorisk research program fund reductions

7981 DUE: 08/31/89 REVISED: COMPLETED:  
Report on Relative Uncertainty of Loading Versus Other Components of Toxic Substances Models

5/88 - title change

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: L104 TOXICS  
ISSUE: J SUPPORT  
PPA (L): 30 TECHNICAL EVALUATION AND ASSESSMENT

PPA (S): TECHNICAL EVALUATION

RC: K ERL ATHNS

PROJECT: 31 Technical Evaluation and Assistance

PROJECT OFFICER: Lee Mulkey

PHONE: FTS-250-3160

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

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PROJECT DESCRIPTION:

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 chemical 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 also will be provided via maintenance of appropriate contracts and liaison with CERL and other Agency support groups. Support, consultation, and assistance to "integrated toxics" projects also will be provided under this project.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

A project was begun to characterize the uncertainty in the estimation of human inhalation exposure to volatile organic compounds (VOCs) associated with domestic water use. The objectives of this project are to construct a model of human inhalation exposure to VOCs from domestic water and to quantify, in a systematic fashion, the uncertainty associated with the modeling process.

The project was initiated in November 1988 with the following tasks completed to date:

1. A literature review to determine what experimentally based data and modeling systems have been developed to date.

2. A model of human exposure (via inhalation) to VOCs from domestic water use (e.g. showers) has been constructed.
3. A Monte Carlo shell (software) has been linked to the model to allow for multiple executions of the model with randomly selected input parameter values.
4. A First Order Error Analysis procedure has been designed for use in the first model.

The project is anticipated to conclude in the coming quarter.

Atmospheric deposition modeling support has been provided for Region V. The objective of this project is to perform a 'screening level' study to determine the contribution of atmospheric deposition to the total mass of toxic pollutants in Lake Michigan. The project was initiated in September 1989 with the following tasks completed during the quarter:

1. Consultation services were provided to Region V to aid in their efforts to write a workplan for constructing a comprehensive toxic emission source inventory.
2. Contacts were made with members of the EPA Atmospheric Research and Exposure Assessment Laboratory (AREAL/Atmospheric Sciences Modeling Division) to establish a cooperative effort for completing the project.
3. In conjunction with AREAL personnel, a draft modeling protocol has been generated.

It is anticipated that the project will continue until the summer of 1989.

STATUS AND SCHEDULE OF DELIVERABLES:

NO DELIVERABLES AVAILABLE

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE  
BUDGET SUB-ACTIVITY: Y105 SUPERFUND  
ISSUE: B EVALUATE TECHNOLOGIES TO MANAGE UNCONTROLLED WASTE SITES  
PPA (L): 02 Biodegradation Applications to Superfund Site Cleanups  
PPA (S): Biodegradation/EPE  
RC: K ERL ATHNS  
PROJECT: 33 Biodegradation Applications to Superfund Site Cleanups  
PROJECT OFFICER: John E. Rogers PHONE: FTS-250-3592  
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PLANNED START: 10/01/88 PLANNED END: 09/01/98  
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PROJECT DESCRIPTION:

GOAL: To evaluate naturally occurring and improved microorganisms for the degradation of hazardous substances under anaerobic and aerobic conditions.

RATIONALE: Increased remedial action activities under the Superfund reauthorization will cause a wide range of cleanup technologies to be evaluated. Biodegradation in some cases, may be the method of choice over chemical and physical remediation. Present knowledge and the availability of biotechnologies for remediation must be expanded to meet this need.

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 the hazardous compound will be enriched from the environment. The key microorganisms in the consortia will be isolated and identified. Environmental parameters that either enhance or inhibit the activity of key organisms will be identified. Methods for moderating or overcoming inhibitory conditions will be developed.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Pentachlorophenol (PCP) is an environmentally toxic chemical that was previously considered recalcitrant to dechlorination under anaerobic conditions. Anaerobic sediments were obtained from a eutrophic lake near Athens, GA; the East River in New York City; and a eutrophic lake in the Soviet Union near the Black Sea. PCP was analyzed by extraction with ethanol and quantitation with HPLC using a C18 reverse phase column.

PCP (20 to 30 ppm) is completely removed within 2 days in sediments acclimated to dechlorinate 10 ppm 2,4- or 3,4-dichlorophenol. Chlorinated intermediate products are concomitantly observed being tetra, tri, di, and mono species with subsequent dechlorination. By contrast, anaerobic freshwater sediments unacclimated to chlorinated phenols require weeks of exposure to PCP before significant degradation and removal of PCP (30 ppm) occurs.

Respiking sediment with PCP results in increased rates of PCP degradation. All degradation rates are apparently first order. Continued respiking eventually results in a slowing of the rate of PCP consumption indicating an inhibitory process.

An abstract, "Dechlorination of Pentachlorophenol in Anaerobic Freshwater Sediments" (Bryant, Howard and Rogers), was submitted for the 1989 ASM Meeting in New Orleans, LA, in May.

STATUS AND SCHEDULE OF DELIVERABLES:

8238 DUE: 10/31/89 REVISED: COMPLETED:  
Report: Potential uses of isolated natural organisms to enhance  
bioremediation of mixed hazardous wastes.

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: Y105 SUPERFUND  
ISSUE: F PROVIDE TECHNICAL SUPPORT TO ENFORCEMENT, PROGRAM & REGIONS  
PPA (L): 22 Enforcement and Other Technical Support/EPE

PPA (S): Technical Support

RC: K ERL ATHNS

PROJECT: 04 Enforcement and Other Technical Support/EPE

PROJECT OFFICER: Donald L. Brockway PHONE: FTS-250-3422

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

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PROJECT DESCRIPTION:

GOAL: Provide tech. support, expert advice, & new methods to Regions assessing exposure/risk at CERCLA sites; emphasize hazard ranking process & subsequent RIFS analysis, particularly ecological risk.

RATIONALE: Exp. assess. and fate multispectral ID techniques for chemicals, databases for environ. properties, & process transform. descriptions are completed or under development. Application to CERCLA ranking & assessment procedures has been limited. Work with Reg. 4/ATSDR will permit immediate use of methods, identify knowledge gaps, and focus study of exposure, health, and environmental assessments.

APPROACH: ERL-Athens, the Regions (via Reg. 4), & ATSDR will identify, develop and demonstrate improved exposure and risk assessments. Improved ecological factors for the hazard ranking system (HRS) will be developed. Case studies will include application of existing ranking methods (HRS), multimedia analysis models, and ecorisk procedures. Results will be used in evaluating existing CERCLA protocols, in transferring technology, and in evaluating need for more research on pollutant fate and exposure/risk assessment. Occurrence of new hazardous source chemicals will be reported to OERR.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

ERL-Athens conducted for OERR/HQ a technical review of the document, "Ecological Assessments of Hazardous Waste Sites." This document was prepared to be a resource to field Superfund personnel involved in ecological assessments, and includes components on assessment approaches, endpoints, toxicity testing, biomarkers, and field surveys. As a resource, the document is thorough but its utility will be limited because of little "how to" guidance in choosing among, for example, the large population of toxicity tests. Review of the document also was obtained from the University of Georgia Institute of Ecology, which is being funded under the Superfund Ecorisk Technology Support Center at ERL-Athens.



The pilot study of results for Tentatively Identified Compounds (TICs) from Superfund Contract Laboratories (CLPs) continues. All of the sample runs from Superfund CLPs have been processed, and data analysis is proceeding. Thirty-five retained extracts and CLP report packages corresponding to many of these runs also have been obtained through the help of the Superfund Sample Management Center. Instrumental runs on the extracts, aimed at identifying those TICs that are of interest, have begun.

STATUS AND SCHEDULE OF DELIVERABLES:

7966 DUE: 02/28/89 REVISED: COMPLETED: 12/31/88  
Report on recommendations for improving the ecological factors of the hazard ranking system  
6/88 - title change

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: Y105 SUPERFUND  
ISSUE: F PROVIDE TECHNICAL SUPPORT TO ENFORCEMENT, PROGRAM & REGIONS  
PPA (L): 22 Enforcement and Other Technical Support/EPE

PPA (S): Technical Support  
RC: K ERL ATHNS

PROJECT: 23 Anaerobic Biotreatment Development/SF

PROJECT OFFICER: John E. Rogers PHONE: FTS-250-3592

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

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PROJECT DESCRIPTION:

GOAL: Characterize and identify basic biological processes that lead to the anaerobic degradation or detoxification of hazardous wastes in contaminated sites.

RATIONALE: A reliable approach is needed for selecting and using 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. Physical and chemical processes affecting the rates also will be characterized. Computer subroutines will be developed to model the processes and effects. The subroutines then will be incorporated into larger computer models for estimating the efficacy of proposed bioremediation processes.

PROJECT STATUS AND ACCOMPLISHMENTS TO DATE:

Information required to adequately evaluate biological treatment proposals targeted for the remediation of hazardous waste sites was defined at a workshop sponsored by the Office of Solid Waste at the Environmental Research Laboratory - Athens on December 13 - 15. Products of the workshop were: (1) a summary of the types of information that would be needed to evaluate the efficiency of a treatment scenario, (2) a list of methods or protocols that could be used for developing the appropriate data, and (3) a list of EPA scientists who could provide assistance to those responsible for evaluating treatment scenarios. Presentations were made by EPA scientists, Dr. J.E. Rogers, ERL-Athens, Dr. J.A. Glaser, RREL-Cincinnati, and Dr. P.H. Pritchard, ERL-Gulf Breeze, and by three university and two industry scientists. EPA attendees came from OSW, OWPE, ORD, and Regions 4, 7, 8, and 10.

Georgia pond sediment enrichments on p-Cresol (pCr) were examined under methanogenic, denitrifying, acetogenic (BESA) and sulfidogenic conditions. Loss of pCr (1 mM) took from three to four weeks in all four

systems. Rate of parent substrate loss in methanogenic cultures was slower than that in denitrifying and acetogenic cultures. Under sulfate reducing conditions pCr was metabolized coincident with 3.3 mM net loss of sulfate, 78% of the theoretical amount. Percent conversion of substrate carbon to gas in methanogenic cultures was 67.7% with 53.9% as CH<sub>4</sub>. Cumulative mmol of CH<sub>4</sub> generated was 89% of the theoretical. Inhibition of CH<sub>4</sub> formation in BESA cultures was incomplete. Acetate was detected only in BESA inhibited cultures. Under denitrifying conditions, stoichiometric conversion to gaseous end products was observed (92.8% of NO<sub>3</sub> was found as N<sub>2</sub> and 5.4% as N<sub>2</sub>O). A transient intermediate, p-hydroxybenzoate was detected, suggesting that pCr metabolism under NO<sub>3</sub><sup>-</sup>/NO<sub>2</sub><sup>-</sup> reducing conditions proceeds through p-hydroxybenzoate and is mediated by a pCr methylhydroxylase as previously shown. These results indicate that pCr is susceptible to degradation under a wide variety of anaerobic conditions. An abstract, "Anaerobic biodegradation of p-Cresol under four reducing conditions" (Rivera, Bossert, Haggblom, Rogers, and Young) was submitted for the 1989 ASM Annual Meeting to be held in New Orleans in May.

#### STATUS AND SCHEDULE OF DELIVERABLES:

NO DELIVERABLES AVAILABLE

FIRST QUARTER STATUS REPORT ON FY'89 PROJECT DESCRIPTIONS  
Office of Environmental Processes and Effects Research  
ERL ATHNS: OCTOBER - DECEMBER 1988

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CODE TITLE

BUDGET SUB-ACTIVITY: Y105 SUPERFUND  
ISSUE: F PROVIDE TECHNICAL SUPPORT TO ENFORCEMENT, PROGRAM & REGIONS  
PPA (L): 22 Enforcement and Other Technical Support/EPE  
  
PPA (S): Technical Support  
RC: K ERL ATHNS  
PROJECT: 29 Center for Exposure Assessment Modeling  
PROJECT OFFICER: Robert Ambrose PHONE: FTS-250-3160

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

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PROJECT DESCRIPTION:

GOAL: Provide regional technical support, expert advice, specialized training, and new methods to conduct exposure assessment modeling for CERCLA sites. To meet ecological impact needs, 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 this technology has been limited because the required highly specialized expertise has not been available or accessible to the Regions and their consultants. Providing a dedicated, operational center for modeling technology will promote 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:

The ORD Center for Exposure Assessment Modeling (CEAM) staff gave several presentations on Superfund projects this quarter. Mr. Ambrose presented "Modeling the Loading, Exposure, and Acute Toxicity of Copper and Zinc in the Upper Clark Fork River" (SETAC); Dr. James Martin presented "Modeling of Confined Disposal Facilities" (SETAC); Dr. Zia Hosseinipour presented "Ground Water Management at Waste Impoundment Sites" (International Conference on Advances in Groundwater Hydrology); Mr. Ambrose presented "Fate and Transport Modeling of Wood Preserving Contaminants in Surface Water" (Forum on Remediation of Wood Preserving Sites); Mr. Ambrose presented a review of CEAM Superfund activities at the Superfund Technology Support Project's fall General Meeting; and

Dr. Martin participated in expert panel review of the Hyde Park/Lake Ontario dioxin modeling study.

Clark Fork River Superfund Site--Developed model network and input data to simulate hydrodynamics and mass transport of metals in Clark Fork River between the Berkeley Pit and Deer Lodge. Prepared and submitted an abstract that discusses the hydraulic model and surface water transport model applications of the Clark Fork River Project to the June 27-30, 1989 Missoula MT, Symposium on Headwaters Hydrology.

Modeling of Confined Disposal Facilities--Completed review and modeling report of the proposed Waukegan Harbor Confined Disposal Facility and submitted to Region 5. Attended meeting November 3 in Grosse Ile MI to present results to state agency and plan for Saginaw Bay studies. Completed literature review of sorption of PCBs on sand filters. Initiated work on revising methods for computing dike transport.

Great Lakes Modeling Activities--Completed review of revised report on modeling of dioxin in Lake Ontario as part of Region II study. Reviewed first draft of dioxin study report by the Large Lakes Research Station and participated in teleconference with other members of expert panel of Hyde Park/Lake Ontario study. Review included verifying model selected computations and predictions.

EcoRisk Support--FCHAIN and FGETS models. Reviewed relevant literature on ecological risk assessment.

Technical Assistance--Provided Robert Hayzen, NJDEP, assistance investigating the problem of on-site human exposure to hexavalent chromium at about 100 hazardous waste sites in New Jersey. Provided Bonnie Eleder, Region V Remedial Project Manager, with a review of the Sheboygan Harbor and River, Wisconsin Remedial Investigation/Feasibility Study Project. Introduced Laura Mazanti, Jeff Stone, Ron Landy, and Judy Sophianapoulos EPA Region IV, to PRZM. Gave demonstration of how to develop input sequence and what parameters are required. Provided Dave Hill, Region IV, advice on use of MINTEQ in predicting lead solubility and speciation at battery cracking superfund sites--Kassouf Kimberling and Flowood. Provided Dave Hill, Region IV, general information and advice on soil cleanup levels targeted for the CSX train wreck site. Provided John Prince, Region II Super RPM for Myers Property Site, NJ, information on potential dioxin risks to humans from contaminated soil and drinking water. Provided Stephen Cipot, Region II, information on the RUSTIC model and training course for possible use at two superfund dry cleaning sites.

Model Distribution--The CEAM Electronic Bulletin Board System (BBS) continued to be well used. Seventy new users registered this quarter, making a total of 389 users. 477 calls were placed to the BBS, and 14 datasets uploaded from users for debugging by CEAM staff. The following exposure models were distributed:

Model	Diskette	BBS	Tape
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WASP4	27	16	0
HSPF9	23	0	3
MINTEQA1	57	3	1
EXAMSII	20	3	2

PRZM	16	11	3
LC50	5	6	0
SARAH	9	1	0
FGETS	13	1	0

Model Support--Continued development, testing, and support of WASP, PRODEF/MINTEQ, and Multimedia models. Began quality assurance/quality control checks and tests of WASP model and support programs and documentation for release of version 4.14 for VAX and PC system implementation, execution, and documentation. Continued migration of CEAM model distribution and registered user data base from VAX to PC environment.

#### STATUS AND SCHEDULE OF DELIVERABLES:

- 8167 DUE: 08/31/89 REVISED: COMPLETED:  
Training Courses for Regional Superfund Staff on Exposure Assessment Modeling
- 8168 DUE: 07/31/89 REVISED: COMPLETED:  
Research Brief on Exposure and EcoRisk Assessments Performed by Center for Exposure Assessment Modeling
- 8169 DUE: 08/31/90 REVISED: COMPLETED:  
Training Courses for Regional Superfund Staff on Exposure Assessment Modeling
- 8170 DUE: 07/31/90 REVISED: COMPLETED:  
Research Brief on Exposure and EcoRisk Assessments Performed by Center for Exposure Assessment Modeling