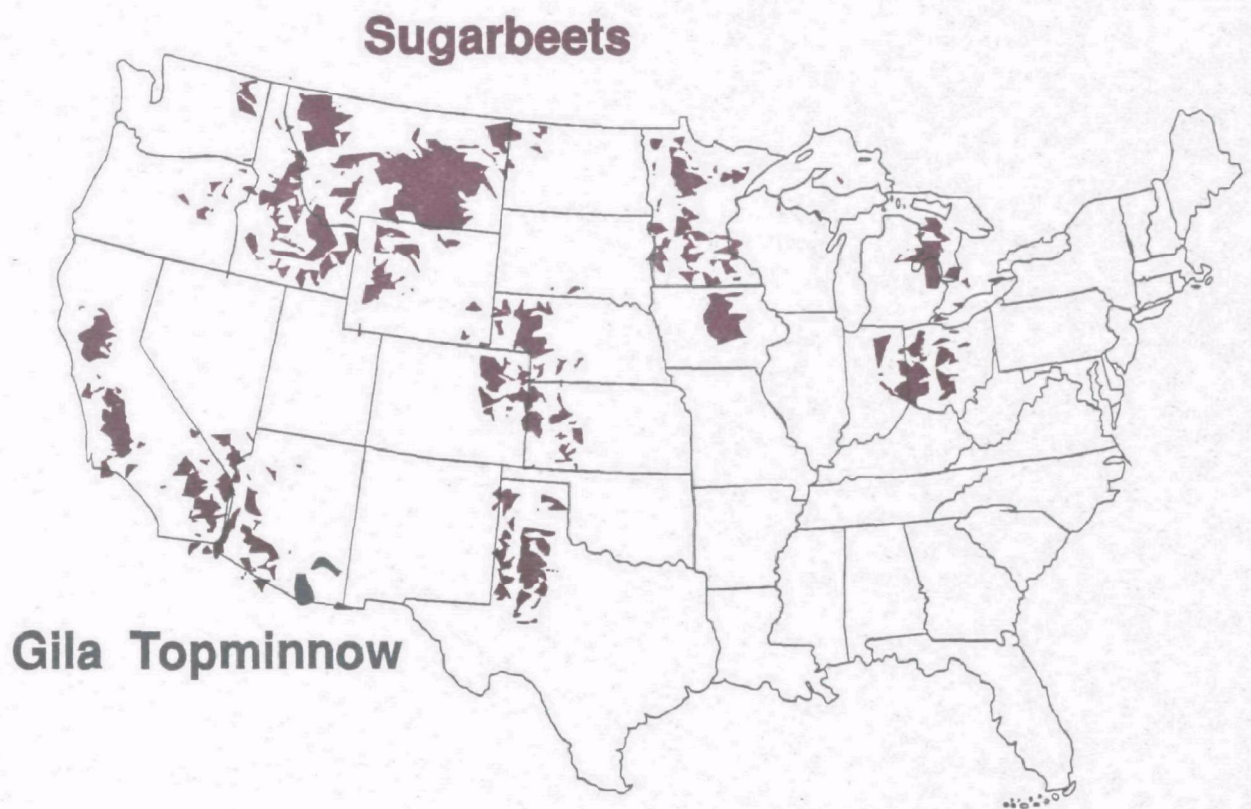




EPA

Environmental Research Laboratory — Athens, GA

1991 Highlights



The U.S. Environmental Protection Agency's Environmental Research Laboratory at Athens, Georgia, conducts and manages basic and applied research to predict, assess, and reduce human and environmental exposures and risks associated with the release of pollutants into freshwater, marine, and terrestrial ecosystems and the emission of greenhouse gases to the atmosphere. The research focuses on predictive environmental fate and exposure and on modeling ecological processes and biospheric system response.

The first focus identifies and characterizes the natural biological and chemical processes in soils, surface waters, and sediments that affect the environmental fate of toxic substances, such as solvents, pesticides, or metals. The results are applied in state-of-the-art multimedia transport models for predicting and assessing exposures and managing environmental pollution problems. The second emphasis involves the development of ecological risk assessment techniques to evaluate pollutant and other stressor effects on ecosystems such as the Great Lakes, Chesapeake Bay, and large agricultural areas.

EPA's Center for Exposure Assessment Modeling (CEAM), an internationally known center for modeling expertise located at the Athens Lab, provides models, training, and support in multimedia exposure evaluation and ecological risk assessment. CEAM assists the Agency and States in environmental risk-based decisions concerning the protection of fresh water, marine water, soil, ground water and air.

Lab-developed fate and process data and assessment techniques support EPA's environmental management regulation and enforcement activities. Major research areas include global climate change, stratospheric ozone depletion, ecological risk assessment, sediment quality evaluation, computational chemistry, identification of complex organic pollutants, nonpoint source pollution management, Environmental Monitoring and Assessment Program (agroecosystems), multimedia nitrogen impacts, bioremediation, chemical remediation, and wellhead protection.

Rosemarie C. Russo, Ph. D., Director

Robert C. Ryans, Technical Information Manager

**Environmental Research Laboratory
U. S. Environmental Protection Agency
960 College Station Road
Athens, GA 30613-0801**

Research Highlights

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ERL-Athens' Multispectral Identification Program Captures Attention of Science Press:

Staff writers for *Analytical Chemistry*, *Environmental Science and Technology*, and *Environment Today* highlight the multispectral identification research program at ERL-Athens to identify unlisted pollutants (or non-target analytes) in samples from the ambient environment. In articles entitled "Multispectral Methods of Analysis and Risk Communication" (*Analytical Chemistry*), "In Search of Something: The 1991 Jekyll Island Meeting" (*Environmental Science and Technology*), and "New Method for Marking Unknown Compounds" (*Environment Today*), journal staff writers address efforts to identify non-target analytes reliably in industrial and municipal wastewaters and samples from Superfund sites. ERL-Athens chemists estimate that conventional identifications of compounds other than target analytes, which are made by computer matching of low resolution electron impact mass spectra, are correct for only about 25% of the chemicals "identified". By elucidating structures on the basis of additional spectral information, the Lab's multispectral identification team can identify, with >99% reliability, compounds that are not even among the ten-million chemicals in the Chemical Abstracts Services Registry. Spectra from high and low resolution chemical ionization mass spectrometry, and Fourier transform infrared spectroscopy are analyzed by the team in an iterative mode to define an unknown

compound's structure. This capability, unique to the Athens Laboratory, opens the door for considering much more comprehensive risk assessments than can be made by addressing only the few hundred priority pollutants and target analytes. Target analytes typically represent less than 2% of the potentially hazardous chemicals in wastewaters and solid wastes.

Lead Speciation, Transport and Bioavailability:

EPA's Office of Research and Development (under the leadership of the Environmental Criteria and Assessment Office) is developing methods to assess human exposure to lead via incidental ingestion of contaminated soils and water. This assessment must take transport and transformation processes into consideration, including the process of lead partitioning between solid (soil) and aqueous phases. The chemical species (form) of lead is significant in terms of its transport and bioavailability, so efforts are underway at the ERL-Athens to predict the occurrence of the various lead species under a variety of environmental and human body conditions. For example, laser spectroscopy is being used to investigate the speciation of lead in blood and to determine the resultant distribution of lead between the two systems. The determination of the speciation of lead in the body and in the environment (e.g., in soil) is tedious and difficult; a complete determination is impossible at this time. A study at ERL-Athens statistically examined the experimentally observed aqueous parti-

DBAPE provides on-line soils and meteorologic data for use with predictive pesticide transport models

...the Lab's multispectral identification team can identify compounds that are not even among the ten-million chemicals in the Chemical Abstracts Services Registry

**Pesticides under
study include
atrazine,
alachlor, and
carbofuran**

**PIRANHA is a
product of the
Ecological Risk
Assessment
Research
Program**

**...laser
spectroscopy
is being used to
investigate the
speciation of
lead in blood**

tioning behavior of lead in 12 aquifer material and sediment samples as a function of pH within the context of 14 sediment chemical/physical properties. A preliminary analysis identifies significant correlations between lead partitioning behavior (i.e., increase in the soil/water lead ratio) and the amounts of sedimentary extractable manganese and particulate organic carbon. The findings from this work, somewhat surprising within the context of conventional geochemistry, will provide direction to future geochemical-speciation-based approaches toward assessing lead mobility in soil systems.

New Fate Constants Database:

A major step has been taken toward elimination of one of the Agency's biggest impediments to comprehensive and quantitative prediction of human health and ecological risks posed by manmade chemicals in the environment. A database developed at ERL-Athens is now online on the laboratory's VAX computer. FATE is the only database of kinetics and equilibrium constants necessary for predicting the fate of chemicals in the environment in which data have been screened for reliability. Scientists using other databases have voiced major concern about the questionable reliability of published fate constants. These concerns arise because quality assurance measures for other databases do not ensure that the data were taken directly from original sources, nor do they incorporate any review to exclude data that were generated under questionable conditions. FATE resolves both of these problems.

The database meets a key Agency need because the lack of reliable fate constants is one of the largest contributor to uncertainty in predicting the risk posed by environmental exposure to manmade chemicals. FATE will assist EPA in its reviews of approximately 4000 chemicals each year for their po-

tential environmental impact and will contribute to the Office of Solid Waste and Emergency Response and the Office of Water in chemical risk assessments.

FATE accommodates data for 12 parameters, and relevant information is also provided to help the user assess the applicability of data for his/her particular purpose. Other features include extrapolation of hydrolysis rates, often measured at elevated temperatures and extreme pH levels, to 25°C and pH 7. Because of the lack of literature data, the questionable reliability of the data, and the prohibitive cost of laboratory measurement, most new data will be computed by SPARC, a highly versatile and reliable computation system under development at ERL-Athens. The FATE database is expected to grow rapidly as SPARC becomes operational for more parameters and broader classes of chemicals.

Predicting Chemical Reactivity by Computer:

The SPARC computer system for predicting reactivity parameters of chemicals strictly from molecular structure is described in an article in the November issue of *Environmental Toxicology and Chemistry*. SPARC uses computational algorithms based on fundamental chemical structure theory to estimate a variety of reactivity parameters (equilibrium/rate constants, UV-visible absorption spectra, octanol/water partition coefficients, etc.) for a broad range of organic compounds. These data are vital for EPA's regulatory activities and can be obtained at a much lower cost using SPARC than by other methods.

Abiotic Reduction Research As Basis for New Chemical Remediation of Contaminated Soils:

Research by Dr. N. Lee Wolfe at ERL-Athens leads to an improved under-

standing of the mechanisms of reduction of a variety of organic pollutants and the environmental conditions under which such processes occur. Nitroaromatics, azo compounds, and some halogenated aliphatic hydrocarbons, for example, are readily reduced to other compounds, which often are less hazardous. Munitions wastes are rich in nitroaromatic organics; reduction of these compounds readily produces aniline derivatives, which can subsequently be aerobically degraded to innocuous products. This could be the basis for simple and effective in-situ chemical remediation technology for the many munitions waste sites in the United States.

Pesticide Transport to Ground Water:

Pesticide residues have been detected in ground water resources in recent years. These findings have fueled new research to better define the extent of the problem, identify key sources and transport pathways, and develop new management alternatives to reduce future degradation of ground water resources. Several research efforts are underway at the Environmental Research Laboratory-Athens to address these problems from the standpoint of developing predictive methodologies for performing exposure/risk assessments, establishing wellhead set-back criteria, and developing information systems for States' use in evaluating management alternatives. Among the 1991 accomplishments were the development of a national database and retrieval system (DBAPE) that provides on-line soils and meteorologic data for use with predictive pesticide transport models. A direct-coupled version of DBAPE and the Pesticide Root Zone Model (PRZM) was produced in the form of the new PRZM Input Collator code (PIC). The DBAPE database also was incorporated into comprehensive assessment modeling methodologies for estimating well-

head setbacks and establishing information systems for States' use in developing pesticide management plans. Critical pesticide transport constructs used in the transport codes are being evaluated under field conditions at a test site in south Georgia.

PIRANHA Adds Components:

Version two of PIRANHA, the Pesticide and Industrial Chemical Risk Analysis and Hazard Assessment Program, is now available. PIRANHA, now in its second year of development in a project coordinated by the ERL-Athens, is a computer-based software system for applying the ecotoxicological and environmental sciences to ecological risk assessment. Version two includes implementation of Department of Agriculture statistics for Major Land Resource Areas, completion of the ichthyofaunal database, major improvements in the Toxicological Inference Program and the PRZM Input Collator program, and a full menu-driven implementation of the model in the VAX CLUSTER environment at the EPA National Computer Center. The final version, planned for delivery in 1995, will encompass analytical capabilities ranging from the estimation of chemical properties from molecular structure through evaluation of risks attending chemical releases to whole ecosystems. PIRANHA is a product of the ORD Ecological Risk Assessment Research Program, which was established in 1985. Environmental contamination by synthetic chemicals is a concern of the Office of Pollution Prevention, Pesticides and Toxic Substances, the Office of Water, the Office of Solid Waste and Emergency Response, and the ten Regional Offices. Five OEPER Environmental Research Laboratories (ERLs) conduct research under the EcoRisk program: ERL-Athens (matrix manager), ERL-Corvallis, ERL-Duluth, ERL-Gulf Breeze, and ERL-Narragansett.

***...chemists
optimized
sample
ionization, while
minimizing
interference
from
matrix ions...***

***FGETS is a
FORTRAN
simulation
model
designed to
predict the
bioaccumulation
of non-
metabolized
organic
chemicals in
fish exploiting
multiple prey
items***

***FATE will assist
EPA in its
reviews of
approximately
4000 chemicals
each year for
their potential
environmental
impact***

***A new model
has been
developed for
analyzing the
discharge of
conventional
and toxic
pollutants from a
multiport
diffuser
into the mixing
zone of a river
or lake***

Pesticide Leaching Database:

A major joint research project among EPA, the Department of Agriculture, the Geological Survey, and the University of Georgia at a field site in Plains, GA, is producing much-needed data on the leaching of pesticides through the soil environment. Pesticides under study include atrazine, alachlor, and carbofuran--all of which are widely used throughout the United States. The comprehensive database is vital to efforts to validate the pesticide leaching models that are frequently used in the regulatory decision process. Validation of models under actual field conditions is cited by the Science Advisory Board and the General Accounting Office as an important Agency need. The database has already been applied in a test of EPA's RUSTIC model.

A Step Closer to Predicting Fate and Transport of Textile Dyes:

Improved methods for the characterization of ten monosulfonated and disulfonated azo dyes resulted from a systematic study using liquid secondary ion mass spectrometry (LSIMS). ERL-Athens chemists optimized sample ionization, while minimizing interference from matrix ions, by studying effects of matrix, primary beam energy, concentration, and mode of operation on the spectra obtained. Approximately 15% of the 250 million pounds of textile dyes used each year in the United States is discharged in the effluents of textile mills. In implementing the National Pollutant Discharge Elimination System, permit writers will eventually have to deal with textile dyes in surface waters, which can result in significant aesthetic deterioration and have caused cancer in laboratory test animals. Comprehensive ecological risk assessments require consideration of the textile dyes

in linking effects of aquatic habitat deterioration to causes. The improved characterization methods will lead to the identification of the dyes and their transformation products in order to predict their transport and transformation in receiving waters.

Model Predicts Bioaccumulation of Chemicals in Fish:

FGETS (Food and Gill Exchange of Toxic Substances) is a FORTRAN simulation model designed to predict the bioaccumulation of nonmetabolized, organic chemicals in fish exploiting multiple prey items. The model can be used by EPA to analyze chemical bioaccumulation in fish species of interest that are exposed to constant or time-varying water concentrations and feed on other fish species, plankton/drift organisms, and/or benthos that also have bioaccumulated the chemicals of concern. In general, the relative contributions of these food items are assumed to be age dependent. The model is supported by its own physiological and morphological database that provides model parameters for important Centrarchids (Lepomis, Micropterus, Pomoxis), Clupeids (Alosa and Dorosoma), Percids (Perca and Stizostedion), Salmonids (Oncorhynchus, Salmo, and Salvelinus), and other selected genera including Catostomus, Cyprinus, Esox, and Ictalurus. This work demonstrates the relative contributions of food chain and direct aqueous exposures are dependent on the particular exposure scenario being considered. This work also shows that the bioaccumulation of extremely hydrophobic chemicals such as the chlorinated dioxins can be predicted assuming that fish insert chemical from contaminated prey and water that is assumed to be in equilibrium with contaminated sediments.

CORMIX2 for Mixing Zone Analysis:

A new model analyzes the discharge of conventional and toxic pollutants from a multiport diffuser into the mixing zone of a river or lake. Called CORMIX2, the model collects the relevant data for the discharge situation, computes the physical parameters, and classifies the discharge into one of many possible hydrodynamic configurations. The model then executes the corresponding hydrodynamic simulation for the flow, interprets the results of the simulation relative to legal requirements including toxic discharge criteria, and suggests possible design alternatives and improvements concerning the mixing characteristics.

Greenhouse Gases and Agriculture:

Agricultural inputs, outputs and wastes that alter atmospheric concentrations of carbon dioxide, methane, and nitrous oxide have been identified. Agriculture ranks third (behind fossil fuel use and chlorofluorocarbon release) among the human activities that can alter the sun-earth energy balance resulting in the potential for climate change. Understanding the net effects of agriculture as a source or sink of greenhouse gases, then, is an important component of EPA's research to understand and control global climate change.

Agriculture ranks third among the human activities that can alter the sun-earth energy balance

Staff Honors and Awards

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Karickhoff Receives SETAC's Highest Award:

The Society of Environmental Toxicology and Chemistry presented its 1991 Founder's Award to Dr. Sam Karickhoff. The society's highest award is presented annually to "a person with an outstanding career who has made clearly identifiable contributions in the environmental sciences consistent with the goals of SETAC." Previous recipients are Dr. Joshua Lederberg, Dr. John Cairns, Jr., Dr. Eugene P. Odum, Dr. Ruth Patrick, Dr. Robert L. Metcalf, Dr. Eugene Kenega, Mr. William D. Ruckelshaus, Dr. Donald I. Mount, Dr. Fumio Matsumura, and Dr. John Sprague.

Dr. Karickhoff is an internationally recognized expert on the sorption of hydrophobic pollutants to sediments. He is the author of numerous articles on chemical sorption and other natural processes affecting pollutant fate in the environment. The Institute for Scientific Information has identified his "Sorption of Hydrophobic Pollutants on Natural Sediments" as a "Citation Classic," one of the most frequently cited works in its field. He received Scientific and Technical Achievement Awards from EPA's Office of Research and Development in 1982, 1985, and 1986.

Dr. Karickhoff's current research offers promise of immense dividends to the

SPARC is applicable to the universe of chemicals providing accurate data required by both EPA and industry for environmental exposure assessments at costs that are much lower than those of conventional data generation techniques

Agency. He is leading a research team to develop a technique for predicting physical and chemical reactivity parameters for modeling the fate of pollutants. The computer-operated system, called SPARC, is applicable to the universe of chemicals providing accurate data required by both EPA and industry for environmental exposure assessments at costs that are much lower than those of conventional data generation techniques.

McCutcheon Named EPA Engineer of the Year:

Dr. Steve McCutcheon was selected as the Agency's Engineer of the Year for 1991. Along with similarly designated engineers from 35 other federal agencies, he will be honored by the National Society of Professional Engineers at an awards ceremony in February 1992. The "Federal Engineer of the Year," as selected by the NSPE from the 35 nominees, will be announced at the awards ceremony. NSPE's Engineer of the Year program, now in its thirteenth year, recognizes the contributions of engineers employed in the Federal government.

Ambrose Garners Bronze Medal:

Mr. Robert Ambrose, Manager of the Center for Exposure Assessment Modeling, has been awarded an EPA Bronze Medal. The award cites his "exceptional leadership in the development, distribution, and support of a system of predictive exposure and risk assessment tools and (his) creative management of the (CEAM)." He was EPA's Engineer of the Year in 1990 and has received Bronze Medals for Commendable Service in 1986 and 1991.

Mulkey Awarded Bronze Medal:

Mr. Lee Mulkey and 12 other members of EPA's Toxicity Characteristics Team were awarded the Agency's Bronze

Medal. The citation reads "For exemplary service resulting in the promulgation of the Toxicity Characteristic, a rule which will help ensure proper management of significant quantities of hazardous waste on a national basis and result in substantial reduction of risk to human health and the environment." EPA calls it the most significant hazardous waste identification rule to be promulgated in the last 8 years.

Garrison, Swank Get Bronze Medal:

Dr. Wayne Garrison and Dr. Robert Swank along with six other members of the Office of Research and Development's MMT Risk Evaluation Team, were awarded the Agency's Bronze Medal for their risk evaluation of a petition by industry to include methylcyclopentadienyl manganese tricarbonyl, an antiknock compound, in unleaded gasoline.

Stancil Awarded Bronze Medal:

Mr. Frank Stancil and six other members of EPA's sediment quality criteria planning committee were awarded an EPA Bronze Medal for their development of the Agency's first five sediment quality criteria standards. Mr. Stancil provided octanol/water partition coefficients for the five chemicals.

Wolfe Garners STAA Award:

The Scientific and Technological Achievement Award Committee presented a Level 3 Award for 1990 to Dr. Lee Wolfe for a journal article, "Characterization of the Reducing Properties of Anaerobic Sediment Slurries Using Redox Indicators," which appeared in *Environmental Toxicology and Chemistry*. Award winners are selected by EPA's Science Advisory Board from nominations provided by all of the Agency's laboratories and offices.

Bailey Elected SSA Chairman:

Dr. George Bailey was elected chairman for 1992-1993 of the Division of Soil Chemistry of the Soil Society of America. The election was the result of voting by the national membership of the Soil Science and Crop Societies of the American Society of Agronomy. This is his second election to a national chairmanship by the ASA. He served as chairman of the Division of Environmental Quality in 1976-1977.

Wolfe Named to International Commission:

Dr. Lee Wolfe was appointed as Titular Member of the International Union of Pure and Applied Chemistry. Among his first duties will be participation in the 36th IUPAC General Assembly in Hamburg, Germany, in May 1992.

Region 9 Thanks Lab for Spill Work:

Dr. Steve McCutcheon, Dr. Larry Burns, Dr. Eric Weber, Mr. Bob Ambrose, and

others at the Lab were cited for their contribution to EPA Region 9 and the State of California in addressing the July 1991 spill of the herbicide metam sodium into the Sacramento River. A letter by Mr. John Wise, Deputy Regional Administrator, to Mr. Erich Bretthauer, AA/ORD, expressed "Region 9's sincere appreciation for the expertise and teamwork provided by ORD's laboratories." He added that the ORD laboratories demonstrated the utmost professionalism in working hand-in-hand with Regional and State agency employees who needed to give guidance to the ongoing response. The letter of appreciation cited the Lab's "effort... on modeling expected concentrations of the herbicide when the spill reached Lake Shasta and its effects on aquatic organisms in the lake; and possible human exposures... and to provide chemical degradation pathways and toxicity information to the Region 9 Water Management Division and to the State of California Governor's Office."

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New Staff and Activities

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Steen Heads Biology Branch:

Dr. William C. Steen was named Chief of the Lab's Biology Branch in August. The announcement was made by Dr. Rosemarie Russo, Lab Director. Dr. Steen, who completed 20 years of Federal service in July (all here at the Athens Lab), manages a branch composed of 27 Federal employees supported by contractor personnel, with a budget of more than \$2 million (internal and

extramural). He has served as acting chief of both the Measurements and Biology Branches and is the US-side chairman of a project under the USA-USSR Agreement on Cooperation in the Field of Environmental Protection with association in two others. He was awarded EPA's Bronze Medal (group) in 1973 and has received two 2% Innovative Research Program funding awards from ORD for special research projects. For the past 3 years, he has served as an Adjunct Professor at the University of Georgia.

**An ERL-Athens
nature trail
project at an
elementary
school was
selected as the
best Partners-
in-Education
Project in
1991 in the
Clarke County
(GA) School
District**

**Four foreign
scientists began
research visits
to ERL-Athens
in 1991**

Weber Receives Innovative Research Funding:

Dr. Eric Weber is one of four OEPER scientists whose innovative research proposals were selected for funding in the FY92 competition. Eric will receive a budget of \$50K for a study of the covalent binding of aromatic amines to humic substances, soils and sediments by ^{15}N NMR.

Garrison Reappointed to Clemson Post:

Dr. Wayne Garrison has accepted reappointment to the position of Adjunct Professor of Environmental Systems Engineering at Clemson University. The appointment is effective for the 1991-1992 academic year.

New Research Geochemist:

Dr. Roger A. Burke, Jr., Research Geochemist, has joined the Chemistry Branch staff. Dr. Burke, who holds a Ph.D. in Marine Science from the University of South Florida, came to the Lab from Texas A&M University; he is involved in global change research concerning stable isotope ratios and flux-emissions of methane from natural wetlands.

New Microbial Ecologist:

Dr. Rochelle Araujo, Microbial Ecologist, joined the Biology Branch staff. Dr. Araujo, who has a Ph.D. in Toxicology from Cornell University, conducts research on the microbial processes that affect chemicals in wetlands and other natural environments.

New Chemist:

Mr. Andrew Paeng, Chemist, joined the Assessment Branch staff. Mr. Paeng, who holds a B.S. in Chemistry from California State University, Bakersfield, performs field studies of chemical movement in soil.

New Research Biologist:

Dr. W. Jack Jones, who holds a Ph.D. in Microbiology from Clemson University, joined the Biology Branch staff. Dr. Jones, who was an associate professor in Georgia Institute of Technology's School of Biology, conducts research in bioremediation, global climate change, and other areas.

International Scientists on Long-Term Visits:

Four foreign scientists began research visits to ERL-Athens in 1991. Ms. Marina Yereschukova of the Hydrochemical Institute of the Russian State Committee on Hydrometeorology and Environmental Protection, began a 9-month study on water quality modeling. Dr. Willie Peijnenburg of the National Institute of Public Health, The Netherlands, completed a 3-month collaborative research project on redox reaction processes. Mr. Hans Bouwers, a graduate student at Wageningen Agricultural University, The Netherlands, completed a 4-month cooperative project on redox reactions of the iron couple with smectite surfaces. Dr. Gokhan Cayci of the University of Ankara, Turkey, began a 6-month cooperative project on pesticide transport and modeling.

Russo Heads Board:

Dr. Rosemarie Russo was reelected as Chairperson of the Agency's Performance Review Board for its Senior Executive Service.

Lab Recognized for Education Program:

An ERL-Athens nature trail project at an elementary school was selected as the best Partners-in-Education project in 1991 in the Clarke County (GA) School District. The nature trail was one of the projects instituted when the Lab adopted the 4th Street Elementary School in a Partners-in-Education Project. Lab staff led trail-clearing ef-

forts on weekends and participated with teachers to develop the trail as a learning tool with curricula and an education booklet to assure that pupils gain maximum education benefit. The Lab staff also conducted an after-school-hours science program and participated in other school programs.

McDaniel Named Science Education Manager:

Ms. Kate McDaniel became the Lab's first Science Education Program Man-

ager in 1991. The appointment reflected the Agency's commitment to the National Environmental Education Act of 1990. In August, the Lab joined with the local chapter of the American Chemical Society to present an environmental science workshop for high school teachers from five area school systems. Emphasis was on environmental chemistry coordinated to help teachers teach science, mathematics, and technology.

Technology Transfer

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Modeling, Training, and On-Site Assistance:

The Center for Exposure Assessment Modeling, EPA's internationally known center of modeling expertise, continued its technology transfer and technical assistance activities in 1991. More than 150 model users from government, industry and academia attended 5 training courses on the QUAL2EU, MINTEQA2, and WASP4 models. In response to requests from the user community, the Center distributed 3379 sets of code for the 22 models it supports. Users also took advantage of the electronic bulletin board to obtain expert help in resolving problems encountered in model application. A total of 3880 bulletin board calls were processed. During the year, 872 new users were added to the CEAM database, bringing the total to 3959 active modelers. CEAM staff continued direct assistance to environmental-problem sites throughout the United States. Staff

provided assistance at 68 Water Program sites, 35 Superfund Program sites, and 9 Resource Conservation and Recovery sites in all 10 EPA Regions.

Symposium on Environmental Analytical Chemistry:

Eighteen invited papers by scientists in government, industry, and university laboratories were presented at the 21st International Symposium on Environmental Analytical Chemistry held on May 20-22 at Jekyll Island, GA. Plenary lectures were presented by Dr. Vincent Covello, Center for Risk Communication, Columbia University; Mr. John Slavick, Chemical Manufacturers Association; and Ms. Ann Cardinal, SRA Technologies, Inc. The symposium also included 31 poster presentations. Approximately 150 scientists from the United States and several foreign countries attended the symposium, which was co-sponsored by EPA.

Workshop on Metal Speciation and Soil Contamination:

Experts from several scientific disciplines participated in a Workshop on Metal Speciation and Contamination of Soil on May 22-24, 1991, at Jekyll Island, GA. Organized by EPA (ERL-Athens), the American Chemical Society, and the University of Delaware, the workshop sought to define the state of knowledge concerning metal chemistry in soil system. The 150 participants included experts in analytical and aquatic chemistry; chemical, civil, environmental, and mining engineering; hydrology; and soil science.

ERL-Athens Scientists at Pittsburgh Conference:

Three scientists from ERL-Athens made major presentations at the 42nd Pittsburgh Conference and Exposition on Analytical Chemistry and Applied Spec-

troscopy on March 4-6. Dr. David Brown discussed the use of equilibrium models in assessing potential environmental problems. Dr. Leo Azarraga reported on metal binding to humic substances as revealed by lanthanide ion probe fluorescence spectrometry. Dr. Lee Wolfe discussed investigations of the redox capacity of anoxic reducing sediments.

International Symposium on Climate Change

More than 30 scientists from the People's Republic of China, the United States, The Philippines, and Canada participated in the International Symposium on Climate-Biosphere Interactions: Biogenic Emissions and Environmental Effects of Climate Change in Beijing in May. The seminar featured presentations by several internationally recognized experts on climatology, biogenic emissions, and the environmental effects of climate change.

Publications in 1991

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Allison, J.D., D.S. Brown and K.J. Novo-Gradac. 1991. MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: Version 3.0 User's Manual. U.S. Environmental Protection Agency, Athens GA. Publication No. EPA/600/3-91/021.

Anon. 1991. Biological Remediation of Contaminated Sediments, with Special Emphasis on the Great Lakes: A Workshop Report. C.T. Jafvert and J.E. Rogers (Eds.). U.S. Environmental Protection Agency, Athens, GA Publication No. EPA/600/9-91/001.

Armstrong, A.Q., R.E. Hodson, H-M. Hwang and D.L. Lewis. 1991. Environmental Factors Affecting Toluene Degradation in Ground Water at a Hazardous Waste Site. *Environmental Toxicology and Chemistry*. 10(2):147-158.

-
- Asmussen, L.E. and C.N. Smith. 1991. Study Design to Investigate and Simulate Agrochemical Movement and Fate in Groundwater Recharge. In: Groundwater Residue Sampling Design. R.G. Nash and A.R. Leslie. (Eds.). Washington DC., American Chemical Society, p. 150-164.
- Banerjee, S. and G.L. Baughman. 1991. Bioconcentration Factors and Lipid Solubility. *Environmental Science and Technology*. 25(3):536-539.
- Barber, M.C., L.A. Suarez and R.R. Lassiter. 1991. Modelling Bioaccumulation of Organic Pollutants in Fish with an Application to PCBs in Lake Ontario Salmonids. *Canadian Journal of Fisheries and Aquatic Science*. 48(2):318-337.
- Baughman, G.L. and E.J. Weber. 1991. Estimation of Water Solubility and Octanol/Water Partition Coefficient of Hydrophobic Dyes. Part I. Relationship between Solubility and Partition Coefficient. *Dyes and Pigments*. 16(4):261-271.
- Bertino, D.J. and R.G. Zepp. 1991. Effects of Solar Radiation on Manganese Oxide Reactions with Selected Organic Compounds. *Environmental Science and Technology* 25(7):1267-1273.
- Bird, S.L., J.M. Cheplick and D.S. Brown. 1991. Preliminary Testing Evaluation and Sensitivity Analysis for the Terrestrial Ecosystem Exposure Assessment Model (TEEAM). U.S. Environmental Protection Agency, Athens, GA. Publication No. EPA/600/3-91/019.
- Brown, K.P., E.Z. Hosseini, J.L. Martin and R.B. Ambrose, Jr.. 1991. Application of a Water Quality Assessment Modeling System at a Superfund Site. U.S. Environmental Protection Agency, Athens GA. Publication No. EPA/600/3-91/046.
- Bryant, F.O., D.D. Hale and J.E. Rogers. 1991. Regiospecific Dechlorination of Pentachlorophenol-Adapted Microorganisms in Freshwater, Anaerobic Sediment Slurries. *Applied and Environmental Microbiology*. 57(8):2293-2301.
- Collette, T.W., R.F. Christman, J.M. McGuire and C.D. Trusty. 1991. Multispectral Identification of Potentially Hazardous Byproducts of Ozonation and Chlorination: Part 1, Studies of Chromatographic and Spectroscopic Properties of MX. U.S. Environmental Protection Agency, Athens, GA. Publication No. EPA/600/4-91/004.
- Donigian, A.S. and W.C. Huber. 1991. Modeling of Nonpoint Source Water Quality in Urban and Non-urban Areas. U.S. Environmental Protection Agency, Athens GA. Publication No. EPA/600/3-91/039.
- Ellington, J.J., C.T. Jafvert, H.P. Kollig, E.J. Weber and N.L. Wolfe. 1991. Chemical-Specific Parameters for Toxicity Characteristic Contaminants. U.S. Environmental Protection Agency, Athens GA. Publication No. EPA/600/3-91/004.
- Grimm, D.M., L.V. Azarraga, L.A. Carreira and W. Susetyo. 1991. Continuous Multiligand Distribution Model Used to Predict the Stability Constant of Cu(II) Metal Complexation with Humic Material from Fluorescence Quenching Data. *Environmental Science and Technology*. 25(8):1427-1431.

- Hale, D.D., J.E. Rogers and J. Wiegel. 1991a. Reductive Dechlorination of Dichlorophenols in Anaerobic Pond Sediment. In: Organic Substances and Sediments in Water. R.A. Baker. (Ed.). Chelsea, MI, Lewis Publishers., p. 211-222.
- Hale, D.D., J.E. Rogers and J. Wiegel. 1991b. Environmental Factors Correlated to Dichlorophenol Dechlorination in Anoxic Freshwater Sediments. *Environmental Toxicology and Chemistry*. 10(10):1255-1265.
- Hayase, K. and R.G. Zepp. 1991. Photolysis of Copper(II)-Amino Acid Complexes in Water. *Environmental Science and Technology* 25(7):1273-1279.
- Hou, M., G.L. Baughman and T.A. Perenich. 1991. Estimation of Water Solubility and Octanol/Water Partition Coefficient of Hydrophobic Dyes. Part II. Reverse-Phase High Performance Liquid Chromatography. *Dyes and Pigments*. 16(4):291-297.
- Imhoff, J.C., R.F. Carsel, J.L. Kittle and P.R., Jr Hummel. 1991. DBAPE—A Database and Model Parameter Analysis System for Agricultural Soils to Support Water Quality Management. *Water Science and Technology*. 24(6):331-337.
- Jafvert, C.T. and J.K. Heath. 1991. Sediment- and Saturated-Soil-Associated Reactions Involving an Anionic Surfactant (Dodecylsulfate). 1. Precipitation and Micelle Formation. *Environmental Science and Technology* 25(6):1031-1038.
- Jafvert, C.T. and E.J. Weber. 1991. Sorption of Ionizable Organic Compounds to Sediments and Soils. U.S. Environmental Protection Agency, Athens GA. Publication No. EPA/600/3-91/017.
- Jafvert, C.T. 1991. Sediment- and Saturated-Soil-Associated Reactions Involving an Anionic Surfactant (Dodecylsulfate). 2. Partition of PAH Compounds among Phases. *Environmental Science and Technology* 25(6):1039-1045.
- Jirka, G.H., R.L. Doneker and T.O. Barnwell. 1991. CORMIX: An Expert System for Mixing Zone Analysis. *Water Science and Technology*. 24(6):267-274.
- Karickhoff, S.W., V.K. McDaniel, C. Melton, A.N. Vellino, D.E. Nute and L.A. Carreira. 1991. Predicting Chemical Reactivity by Computer. *Environmental Toxicology and Chemistry*. 10(11):1405-1416.
- Kolig, H.P. and J.J. Ellington. 1991. Fate Constants for Some Chlorofluorocarbon Substitutes. U.S. Environmental Protection Agency, Athens GA. Publication No. EPA/600/M-91/007.
- Kolig, H.P., K.J. Hamrick and B.E. Kitchens. 1991. FATE, the Environmental Fate Constants Information System Database. U.S. Environmental Protection Agency, Athens GA. Publication No. EPA/600/3-91/045.
- Lewis, D.L. and D.K. Gattie. 1991a. Predicting Chemical Concentration Effects on Transformation Rates of Dissolved Organics by Complex Microbial Assemblages. *Ecological Modeling*. 55(1/2):27-46.
- Lewis, D.L. and D.K. Gattie. 1991b. The Ecology of Quiescent Microbes. *ASM News*. 57(1):27-32.

-
- Loux, N.T., J.D. Allison, C.R. Chafin and S.M. Hassan. 1991. Carbonate Equilibria and Groundwater Sample Collection: Implications for Estimated Average Subsurface Properties in Continental North America. *International Journal of Environmental Analytical Chemistry*. 44(1):41-53.
- Mueller, T.C., P.A. Banks and W.C. Steen. 1991. Microbial Degradation of Flurtamone in Three Georgia Soils. *Weed Science*. 39(2):270-274.
- Richardson, S.D., A.D. Thruston, Jr., T.W. Collette and J.M. McGuire. 1991. Application of Multispectral Techniques to the Precise Identification of Aldehydes in the Environment. *Environmental Toxicology and Chemistry*. 10(8):991-997.
- Richardson, S.D., A.D. Thruston, Jr., J.M. McGuire and G.L. Baughman. 1991. Influence of Experimental Conditions on the Liquid Secondary Ion Mass Spectra of Sulfonated Azo Dyes. *Organic Mass Spectrometry*. 26(10):826-830.
- Said, W.A. and D.L. Lewis. 1991. Quantitative Assessment of the Effects of Metals on Microbial Degradation of Organic Chemicals. *Applied and Environmental Microbiology*. 57(5):1498-1503.
- Steen, W.C. 1991. Microbial Transformation Rate Constants of Structurally Diverse Man-made Chemicals. U.S. Environmental Protection Agency, Athens GA. Publication No. EPA/600/3-91/016.
- Susetyo, W., L.A. Carreira, L.V. Azarraga and D.M. Grimm. 1991. Fluorescence Techniques for Metal-Humic Interactions. *Fresenius' Journal of Analytical Chemistry*. 339(9):624-635.
- Thruston, A.D., Jr., S.D. Richardson, J.M. McGuire and T.W. Collette. 1991. Multispectral Identification of Alkyl and Chloroalkyl Phosphates from an Industrial Effluent. *Journal of American Society for Mass Spectrometry*. 2(5):419-426.
- Trusty, C.D. and J.J. Ellington. 1991. Techniques Affecting Precision and Accuracy in Hydrolysis Rate Constant Determinations of Volatile Organic Compounds Using Jeffers' Zero Headspace Reaction Bulbs. *Analytical Letters*. 24(2):327-344.
- Weber, E.J. 1991. Studies of Benzidine-based Dyes in Sediments-water Systems. *Environmental Toxicology and Chemistry*. 10(5):609-618.
- Wolf, S.D., R.R. Lassiter and S.E. Wooten. 1991. Predicting Chemical Accumulation in Shoots of Aquatic Plants. *Environmental Toxicology and Chemistry*. 10(5):665-680.
- Yen, C-P.C., T.A. Perenich and G.L. Baughman. 1991. Fate of Commercial Disperse Dyes in Sediments. *Environmental Toxicology and Chemistry*. 10(8):1009-1017.
- Zepp, R.G. 1991. Photochemical Fate of Agrochemicals in Natural Waters. In: *Pesticide Chemistry: Advances in International Research, Development, and Legislation*. H. Frehse. (Ed.). Weinheim (Germany), VHS, p. 329-345.