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SOUTH CAROLINA DOE/EPSCoR ENERGY-RELATED GRADUATE RESEARCH TRAINEESHIPS

Final Report

and

Progress Performance Report

for period

January 1, 1995 - December 31, 1995

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DISCLAIMER

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A. SUMMARY OF PROGRESS

1. Recruitment/Response/Selection of Trainees

The South Carolina DOE/EPSCoR Graduate Traineeship Program was granted a no-cost extension for the period September 30, 1993 through December 31, 1995. Eleven new students were funded for the report period of January 1, 1995 - December 31, 1995 and nine students, previously supported, were continued.

All graduate students in appropriate academic disciplines are made aware of the existence of the DOE/EPSCoR Traineeship Program but are not considered for a traineeship unless they have completed at least one academic semester of graduate school. Faculty who have at least part of their research focused into an energy-related project (key faculty) are identified in the initial proposal and include not only those with active funding, but also past funding and significant publications in an energy related area. These faculty serve to identify new trainee candidates and are from the following institutions and departments:

Clemson University (CU) Chemistry, Computer Science, Engineering, Mathematics, Physics.

Medical University of South Carolina (MUSC) Biostatistics/Epidemiology, Microbiology & Immunology, Opthamology/Biochemistry, Pharmacology.

University of South Carolina (USC) Biological Sciences, Chemistry & Biochemistry, Computer Science, Geology, Chemical & Mechanical Engineering, Mathematics, Physics & Astronomy, Statistics.

The following state EPSCoR committee members meet to make final selection or decisions regarding continued support of the trainees:

Rosalie Crouch, Dean, MUSC, College of Graduate Studies
Jerome D. Odom, Dean, USC, College of Science & Mathematics
Thomas M. Keinath, Dean, CU, College of Engineering and Science
Chris Przirembel, Accociate Dean for Research, CU, College of Engineering and Science

A summary of the new trainees appointed during this report period, and those for which support was continued, is provided in table 1.

TABLE 1
1995 DOE/EPSCoR Graduate Research Trainees[a]

NAME	GPA	INSTITUTION DEPARTMENT	ADVISOR	RESEARCH AREA	Ph.D. DATE	THESIS TITLE	PRACTICUM AGREEMENTS
Bradley Johnson	3.3	USC / Chemical Engineering	R. E. White	Lithium Ion Batteries	5/97	The Mathematical Modeling of a Lithium Ion Battery System	Hoechst Celeanese Corporation Contact: Dr. Robert Sportnitz (704-587-8537)
Christopher Bunker	4.0	Clemson / Chemistry	Y. Sun	Analytical Chemistry/Spectroscopy of Polymer Films	5/97	Experimental and Computational Studies of Complicated Chemical Systems	None reported at date of report
Steven Christopher	3.7	Clemson / Chemistry	R. K. Marcus	Analytical Chemistry/Mass Spectrometry	5/97	Ion Kinetics and Detection of Radio Frequency Glow Discharge Generated Ions	CID Technologies
Patrick Joyce	3.0	Clemson / Chemical Engineering	M. C. Thies	Supercritical Fluid Extraction	12/98	Separation of Fischer-Tropsch Wax from Catalyst using Supercritical Fluid Extraction	None reported at date of report
Scott Brame	3.7	Clemson / Geological Sciences	D. S. Snipes	Multiphase Flow Remediation	12/98	The Relationship of Aquifer and Contaminant Characterization to the Success of Specific Remediation Technologies	Westinghouse Savannah River Company
Stewart Edmunds	3.7	MUSC / Marine Biomedical and Environmental Sciences	J. S. Ramsdell	Estrogenic Contaminants	12/98	The Effect of Complex Mixtures of Estrogenic Contaminants on Sexual Differention in Finfish	NOAA Southeast Fisheries Science Laboratory Contact: Dr. Sylvia Galloway (Director) 803-762-8617
Albrecht Carver	4.0	Clemson / Electrical and Computer Engineering	R. J. Schalkoff	Autonomous Robotic Inspection System	5/97	Model Based Photometric Stereo	None reported at date of report
James Roane	4.0	Clemson / Environmental Systems Engineering	R. A. Fjeld	Transuranics and Beta Emitters	5/98	Measurement of Radionuclides in Environmental and Waste Samples using Ion Chromatography and Flow-Cell Scintillation Counting	Rust Federal Services, Clemson Technical Center Contact: Dr. John Leyba (864) 646-2413
Shawn White	3.8	Clemson / Chemistry	R. R. Williams	Spectroscopy	12/97	Development of a Miniature Fiber Optic Spectrometer	Westinghouse Savannah River Company
Wendy Bell	3.7	USC / Chemistry and Biochemistry	M. L. Myrick	Organic Waste Disposal	8/97	In-situ Raman Spectroscopy of Organic reactions in Supercritical Water	Eastman Chemical Company Contact: Mike Cushman (615) 229-4075
Samuel Brown	3.1	USC / Chemistry and Biochemistry	S. M Angel	Fiber-Optic Sensors	5/96	Low Temperature Raman Cell for Improved Detection of Solvent Vapors	Lawrence Livermore National Laboratory Contact: Dr. Fred Milanovich (510) 422-6838

[a]Abbreviations used: USC, University of South Carolina; MUSC, Medical University of South Carolina

(Table continued on following page)

TABLE 1 (CONT.)
1995 DOE/EPSCoR Graduate Research Trainees

Phillip Levine	4.0	USC / Geological Sciences	C. Kendall	Sediment Computer Modeling	12/96	Sequence Stratigraphic Interpretation and Modeling of Permian Depositional Systems, Vacuum-Abo Field, Lea County, New Mexico	Amoco Production Company Contact: Dr. Susan Nissen (918) 660-3518
Christopher Murray	3.9	USC/ Geological Sciences	R. Ehrlich	Groundwater Geochemical Data Analyses	5/96	The Use of Nuclear Magnetic Resonance T(2) Distributions to Characterize the Porous Microstructure of Sand-stones	Savannah River Company June-September 1993
Ray S. Williams	4.0	USC/Biology	D. E. Lincoln	Rising CO_2 Effects on Plant/Insect Interactions	8/95	Herbivorous Insect Responses to Elevated CO(2) Grown Tree Species	Oak Ridge National Laboratory April-July 1993
James B. Robb II	3.7	USC/Chemistry	J. R. Durig	Molecular Structure of Organophosphorus Compounds	8/96	Conformational Analysis by Infrared and Raman Spectroscopy and *Ab Initio* Calculations of Some Environmentally Important Organophosphorous Compounds	Savannah River Company Summer 1994
Edward M. Stack	3.8	USC/ Geological Sciences	A. Cohen	Environmental Geology	12/95	Extraction Potential of Peats for Various Hazardous Waste Substances	Argonne National Laboratory June-Dec (1992) & Oct-Dec (1993)
G. Lopez-de-Victoria	3.8	USC/Biological Sciences	C.R. Lovell	Bioremediation	12/95	Motility and Chemotaxis of Azospirillum	Savannah River Company[b]
Derek Sanders	3.6	USC/Computer Science	R.L. Cannon	Sediment Computer Modeling	5/96	The 3-D Interpolation of Surfaces and Volumes Within a Fence Diagram of 2-D SEDPAK Generated Cross-Sections	Texaco Contact: T. L. Burnett (713) 432-6808
Istvan Csato	3.8	USC / Geology and Marine Science	C. Kendall	Sediment Computer Modeling	12/95	Sequence Stratigraphic Interpretations and Modeling in Lacustrine Rift Basins - Southern Dead Sea Basin, Israel and Pannonian Basin, Hungary.	Texaco Research Center Contact: Dr. Garry Proddy (713) 954-6018
Sean R. Ryan	3.9	USC / Geological Sciences	C. Kendall	Stratigraphic Modeling	5/96	Depositional Sequence Analysis and Stratigraphic Simulation of the Aptian/Albian Torok and Nanushuk Formations, National Petroleum Reserve, North Slope of Alaska: in press with the program of the Annual Meeting for the American Association of Petroleum Geologists	Alaskan Division of Oil and Gas Contact: Dr. Tim Ryherd (907) 762-2140

[b]Practicum arrangements canceled due to unexpected pregnancy

B. SUMMARY OF RESEARCH ACTIVITIES/EFFORTS PERFORMED

Bradley Johnson
Department of Chemical Engineering
University of South Carolina
Dissertation Advisor: R. E. White
Research Area: Lithium Ion Batteries

The overall objective of the research performed through the DOE/EPSCoR Traineeship Program is to develop a performance model for the lithium ion battery system. Working with Hoechst Celanese Corporation's Separations Products Division in Charlotte, North Carolina, Mr. Johnson was well equipped to perform studies necessary to meet this objective.

In order to develop a robust performance model for this relatively new technology, it is necessary to thoroughly understand the system. This task was accomplished through a comprehensive characterization of commercially available cells. Both Sony and Matsushita (Panasonic) cells were characterized. This process included performing cell dissections, rate studies, self-discharge studies, temperature effect studies, and cycle-lifetime studies. The cell dissections proved to be a valuable tool in learning about the cell's operation as well as the safety mechanisms employed in this highly reactive battery system. Several design differences between the Sony and Matsushita cells were noted. The other studies of commercial cells served as good comparisons between the two systems and more importantly, gave data by which the performance model can be validated. The components of this task were performed continuously over the entire time period of the traineeship. A short summary of this work showed that the two design types used different anode materials. The Sony cell used coke, while the Matsushita cell used a form of graphite. In addition, the performance of the Matsushita cell seemed to be superior to the Sony cell in every aspect measured. The Matsushita cell performed with a higher efficiency at high discharge rates and low temperatures, as well as having a higher cycle-lifetime and energy density. Despite this fact, Sony cells dominate the lithium ion market.

A second task which was started during this time period involved experimental studies of a lithium ion battery system. An apparatus was designed, assembled, and tested over a four month time frame.

The goal of these experiments was to develop a protocol for constructing reproducible electrodes for the lithium ion battery system. This task was aided by a visit to the Arthur D. Little Company in Cambridge, Massachusetts.

The work performed under the DOE/EPSCoR Traineeship program provided important background data for the advancement of experiments necessary to provide model parameters. The work performed has proven valuable both to the completion of my thesis project and to Hoechst Celanese Corporation's Separations Products Division.

Christopher Bunker
Department of Chemistry
Clemson University
Dissertation Advisor: Y. P. Sun
Research Area: Analytical Chemistry/Spectroscopy of Polymer Films

During this report period, Mr. Bunker has been carrying out a research project concerning the probing of microstructures and properties of polyelectrolyte membranes by use of luminescence spectroscopic methods.

In the first month of the project, Mr. Bunker, with the help of machine shop staff, constructed a solid sample holder for luminescence spectrometers. The sample holder was specifically designed by Mr. Bunker for the study of polyelectrolyte membranes. He also made a series of modifications to a set up for time-resolved luminescence measurements, so that the instrument would be more suited to the studies required by the project. His efforts were successful.

During two months of the report period Mr. Bunker was trained by Dr. J. J. Ma to treat a commercially available polyelectrolyte membrane, Nafion, which serves as the reference for investigations of other polyelectrolyte membranes. Following his training, he managed to prepare Nafion films in both acid and sodium forms for spectroscopic studies. He made preliminary spectroscopic measurements of two fluorescent molecular probes pyrene and p-N,N-dimethylaminobenzonitrile (DMABN) in Nafion films, and obtained some interesting and significant results. It was found that pyrene behaves very differently in a Nafion film from in a bulk aqueous solution. As well established in the literature, pyrene is widely used as fluorescent probe for measuring the microscopic polarity of the medium environment. The ratio of the first and the third vibrational bands in the pyrene fluorescence spectrum is strongly polarity-dependent. The ratio is often referred to as the Py polarity scale. For pyrene in Nafion membrane, the observed fluorescence spectra show that the local medium environment is much less polar than that in an aqueous solution.

DMABN is another fluorescent molecular probe that is known to respond to medium polarity sensitively. Mr. Bunker's results show that the behavior of DMABN is dramatically different in acid and sodium forms of Nafion membranes. In the acid form, the probe molecule is exclusively protonated, which changes the spectroscopic properties of the molecule completely. In the sodium form, however, the observed fluorescence spectra again show that the microscopic environment in Nafion film is less polar than that in a bulk aqueous solution. It seems that the two different kinds of molecular probes yielded consistent results.

Mr. Bunker also did a survey of literature results on spectroscopic studies of polyelectrolytes. It provided him with important training in the critical evaluation and the use of literature information in his research.

Steven Christopher
Department of Chemistry
Clemson University
Dissertation Advisor: R. K. Marcus
Research Area: Analytical Chemistry/Mass Spectrometry

Over the report period, studies have been undertaken which involve the direct imaging of glow discharge-generated ions with a charge injection device (CID) detector. The driving force behind this research stemmed from a discovery at the Savannah River Westinghouse Technology Center, which found the CID to be responsive to ions.

The project involved constructing a dedicated vacuum system for ion imaging experiments. The first ion imaging system consisted of a radio frequency glow discharge source interfaced to a modified Hewlett-Packard (HP-5985) vacuum chamber. Located inside the chamber were two ion optic lenses, a Faraday cup detector, and the CID. The Faraday cup was mounted on a moveable probe and could be placed in the ion beam path (for ion beam current measurements), or retracted to facilitate CID ion imaging. Ion images obtained with the above ion optic configuration showed the CID to be responsive to plasma ions and photons.

Although the software that operates the CID allows for the background subtraction of images, the complete elimination of plasma photon contribution would be preferred. This led to the development of a second ion optic configuration. Ion images were successfully obtained in the complete absence of photons. Preliminary ion trajectory and kinetic energy simulations showed that the CID was responsive to approximately 30eV ions. Furthermore, the data showed that there was a kinetic energy threshold that had to be met prior to an image being registered on the device.

Both of the above ion optic configurations suffered from physical restrictions of the vacuum chamber and no attempt was made to optimize ion lens dimensions or their distances with respect to the CID. Also, CID operation over extended periods of time suffered from an insufficient cooling probe that rested on the backside of the device. With no mechanism for heat loss under high vacuum, CID dark current rapidly increased as a function of time. Finally, the exact energy required to register an image could not be measured with either configuration.

All of the above considerations led to the development of what is envisioned as the final (current) ion imaging system. An entirely new vacuum system was developed to house an electrostatic energy analyzer (ESA) to facilitate controlled energy studies. A more efficient cooling system was also designed to minimize CID dark current. Investigations of the response of the CID to ions of various energy are currently underway. CID imagers possessing different protective glass passivation layer thicknesses and ion-sensitive epitaxial layers are also being evaluated. At this point, the mechanism for charge production in the devices is undetermined but is most likely caused by a combination of translational and potential energy effects, and will clearly be dependent on the thickness of the imager's protective glass layer.

Patrick Joyce
Department of Chemical Engineering
Clemson University
Dissertation Advisor: M. C. Thies
Research Area: Supercritical Fluid Extraction

The objective of this research project is to evaluate the potential of SCF extraction for separating the catalyst slurry of a Fischer-Tropsch (F-T) slurry bubble column (SBC) reactor into two fractions: (1) a catalyst-free wax containing less than 10 ppm particulate matter and (2) a concentrated catalyst slurry that is ready for recycle or regeneration. The wax will be extracted with a hydrocarbon solvent that has a critical temperature near the operating temperature of the SBC reactor, i.e., 200-300 °C.

During the support period, work on the small-scale, continuous-flow apparatus continued. All system leaks have been located and eliminated. The differential thermocouple circuits that existed in the nitrogen bath were found to be faulty, possibly due to oxidation of the copper wires, and have been rebuilt. Initial experiments have been performed on a binary mixture of n-hexane (solvent) and squalane (model compound) at 473 K, the lower temperature limit of a SBC reactor. A total of fifteen runs were completed at 135, 160, and 208 psig, with pressures being controlled to within ± 2 psi. Results indicate that the equilibrium phase compositions can in principle be measured to a reproducibility of better than ±0.5% in the squalane-rich bottom phase and to ±2% in the hexane-rich top phase. For example, a bottom-phase composition of 57.0±0.1 wt % squalane was measured at 160±2 psig and 200.50±0.10 °C for 3 consecutive samples. Similarly, the top phase was found to contain 0.0475±O.0005 wt % squalane in 3 samples collected at the same conditions. However, other data measured at these same conditions at another time exhibited scatter that was as much as 5 times greater. We believe that improvements in (1) the method of preheating the feed to the view cell/phase separator and to (2) the sample collection technique are required before data of high quality can consistently be generated. The apparatus modifications required to effect these improvements arc currently underway and should be completed by the middle of the month.

Scott Brame
Department of Geological Sciences
Clemson University
Dissertation Advisor: D. S. Snipes
Research Area: Multiphase Flow Remediation

Mr. Brame conducted and analyzed pump tests to determine hydraulic conductivities of aquifers for the USGS Savannah River Underflow project. This data is being used to determine if contaminants have the potential to travel from the Savannah River site under the river into Georgia. As part of this project Mr. Brame worked with another student to determine rates of leakage between the primary aquifers through the confining layers using numerical simulations. The models used were MODFLOW and its radial version, RADMOD.

Mr. Brame condensed and edited a thesis by David Kroening that dealt with rehabilitation of wells clogged at the Savannah River Site. The final form of the paper was accepted for publication this spring or summer in the journal *Groundwater Monitoring and Remediation*.

Mr. Brame investigated the potential for cleaning up sites that have groundwater contaminated with non-aqueous phase liquids (NAPLs). This research involved both lighter than water organic contaminants (LNAPLs) and denser than water organic contaminants (DNAPLs). The research was conducted with lab experiments and using multiphase, multicomponent numerical simulations. Much of this work was geared toward the application to a field site. The specific aspects studied included partitioning tracers for determining residual saturations, effects of different cosolvents on NAPL dissolution and mobilization, and the stability of chemical fronts through porous media. Much of this work was conducted in conjunction with the Environmental Systems Engineering Department at Clemson.

Stewart Edmunds
Department of Marine, Biomedical and Environmental Sciences
Medical University of South Carolina
Dissertation Advisor: J. S. Ramsdell
Research Area: Estrogenic Contaminants

Mr. Edmunds conducted experiments to develop a reporter gene assay for estrogenic contaminants and initiated experiments to examine several different classes of contaminants for estrogenic activity with this new methodology.

A variety of environmental contaminants have been implicated to adversely effect humans and wildlife through interaction with the endocrine system and have been broadly defined as environmental endocrine disrupters. Estrogen pathways controlling sexual development and differentiation are among the most susceptible endocrine targets. Although assays using receptor binding or cell proliferation have been developed, a need exists for an assay that directly asseses effects on estrogen responsive gene activity and one that is sensitive, rapid and capable of analyzing large data sets.

The estrogen response element from Xenopus vitellogenin A2 was ligated to the luc reporter element from firefly luciferase. This construct was then introduced into an estrogen responsive cell line (GH4C1) together with a plasmid containing the neo gene that confers gentamyicin resistance. Clonal cells were isolated as resistant to gentamycin and then screened for luciferase activity. Several clones were grown to mass culture and one clone was selected for further study based on estrogen induction of luciferase.

A simple assay was developed to detect estrogen activity and sensitivity to estrogen was determined. 17β-estradiol induced luciferase activity with an EC_{50} of $6.5 \pm 2.4 \times 10^{-11} M$. This sensitivity was well within the range necessary for analysis.

Natural and synthetic hormones were examined for activity. Dexamethasone, aldosterone, and thyroxine did not induce luciferase activity, whereas 10^{-8}M diethylstilbestrol and 10^{-5}M trans-retinoic acid (RA) induced luciferase activity equal to 17β-estradiol, indicating that transcription of the luciferase gene is primarily regulated through the endogenous estrogen and RA receptors. Two classes of pesticides were examined for activity. The pesticide o,p'-DDT and endosulfan were found to be estrogenic at concentrations as low as 10^{-7}M. Three PCB's were examined for activity. 2',4',6'-trichlorobiphenyl and its hydroxylated metabolite 40H-2',4'.6'-trichlorobiphenyl were estrogenic at 10^{-7}M, whereas 2,4,4'-trichlorobiphenyl did not induce luciferase activity.

Lastly the GH_4C_1 ERE-Luc reporter gene assay was modified to use a cell permeant luciferin. The assay was then modified to run in 96 well microplates through the entire procedure from administration of contaminants to the detection of light emission This modification involves far fewer technical manipulations during the assay procedure and thus permits the screening of multiple and complex samples in a cost effective manner.

Albrecht Carver
Department of Electrical and Computer Engineering
Clemson University
Dissertation Advisor: R. J. Schalkoff
Research Area: Autonomous Robotic Inspection System

In the period January 1995 through December 1995, Albrecht Carver was involved in the development of the vision system for the ARIES (Autonomous Robotic Inspection Experimental System). The system is being developed for the Department of Energy to survey and inspect drums containing low-level radioactive waste stored -in warehouses at DOE facilities. The system, on the basis of visual information, makes autonomous decisions about the condition of the drums, including location of any unique visual features, characterization of relevant surface features of interest (such as paint blisters, rused areas etc.), and updating a database containing the inspection data. Mr. Carver was involved in all aspects of the development of the ARIES vision system, however his major contributions were in the physical design of the vision system, the development of the techniques needed for finding and isolating the drum in an image, and the physical and algorithmic implementation of the system.

Due to warehouse imaging conditions, segmentation of the imaged drum from the scene background (which consists of, among other entities, other similar drums) is a challenging task. Traditional edge extraction and region segmentation techniques fail due to a variety of non-ideal working conditions (glossy drums, multiple reflections, gradual fading of intensity, etc.). This justified using structured light, specifically five laser dots, to ascertain the drum size, range, and horizontal location. The vertical edges of the drum in the image are found via simple geometry and the perspective-projective transform. The vertical extent of the drum in the image is determined by finding the drum-shaped region which maximizes a color contrast metric.

Another aspect of the drum segmentation is the exclusion of regions on the drum which are not to be analyzed for rust or blisters. These regions are paper labels such as bar-codes and warning signs typically found on stored drums, The diffuse reflections from paper is typically much greater than that from paint. Since diffuse reflections are direction insensitive, the paper is segmented from the drum by finding regions which exhibit less change in intensity when the lighting direction is changed.

James Roane
Department of Environmental and Systems Engineering
Clemson University
Disssertation Advisor: R. A. Fjeld
Research Area: Transuranics and Beta Emitters

Radiological characterization and monitoring is an important component of environmental management activities throughout the Department of Energy complex. Radionuclides which cannot be detected by gamma-ray spectroscopy, such as pure beta emitters and transuranics, pose special problems because their determination generally requires labor intensive radiochemical separations procedures that are time consuming and not practical for field applications.

This project is focused on a technology that can measure transuranics and pure beta emitters relatively quickly and has the potential of being field-deployable. This technology combines high performance liquid chromatography and on-line scintillation counting with alpha/beta pulse shape discrimination. In previous studies, the ability to measure pure beta emitters such as ^{63}Ni, ^{90}Sr, and ^{99}Tc, and actinides/transuranics such as ^{232}Th, ^{233}U, ^{237}Np, ^{239}Pu, ^{241}Am, and ^{241}Cm was demonstrated. However, the previous work was primarily limited to aqueous samples of relatively high purity and to radionuclide concentrations that are representative of many waste applications, but are higher than those typically encountered in environmental cleanup applications. The goal of the current project is to apply the technique to complex matrices such as sludge and soil at radionuclide concentrations typical of environmental samples. Consequently, the objectives of the current project are (1) to develop sample processing protocols to remove chemical and radiological interferences from complex matrices and (2) to lower detection limits. During the fellowship period, the experimental apparatus was assembled, a standard was developed for routine checks of system performance, and radiological interference studies were performed for natural thorium, natural uranium, ^{228}Th, ^{137}Cs, ^{60}Co, and ^{3}H.

Shawn White
Department of Chemistry
Clemson University
Dissertation Advisor: R. R. Williams
Research Area: Spectroscopy

The research conducted focused on spectroscopic analysis of various indicator dyes in a supercritical bomb. The visible absorbance data were acquired using an Ocean Optics S1000 fiber optic spectrometer run by a 16-bit microcontroller. A tungsten-halogen lamp with fiber optic couplings was used as the source. Seven mL of the indicator solution was injected into the stainless steel bomb that had a total volume of 10 mL. After placing the bomb in an oven heating element spectra of the bomb were taken every five minutes. Each spectrum at each time consists of 50 scans averaged together. The single beam spectra of the indicator solution were normalized against the spectrum of water in the bomb at room temperature to give transmittance spectra. The indicator solution was a 13.8 mM aqueous solution of various indicator dyes including bromothymol blue, cresol red, and phenol red. The decrease in absorbance is most probably a result of a decrease in concentration of the dye species caused by thermal or chemical degradation of such severity little information about the chemical environment of the bomb can be gained from these labile species.

Wendy Bell
Department of Chemistry and Biochemistry
University of South Carolina
Dissertation Advisor: M. L. Myrick
Research Area: Organic Waste Disposal

Environmental concerns are making the safe disposal of organic wastes extremely difficult. One means of alleviating the problem is to develop new synthetic methodologies which utilize non-hazardous reactants or solvents. Water is the most environmentally benign solvent but its use has been limited by its inability to dissolve most organic compounds. This disadvantage can be overcome by the use of supercritical water as a reaction medium. Despite the potential usefulness of supercritical water in both synthetic and destructive organic reactions, very little is known about the fundamental chemistry of reactions in supercritical water. Clearly the chemistry in such a medium will be quite different from normal conditions, but at this point very few investigations have been carried out.

One problem with understanding the chemistry in supercritical water is the lack of spectroscopic probes to monitor reactions due to the challenges posed by the high temperatures and pressures (375 C, 3500 psi), as well as the highly corrosive nature of supercritical water. Raman spectroscopy is an almost ideal technique for probing organic reactions in supercritical water due to the weak scattering observed for water itself, as well as the highly polarizable nature of most small organic molecules. In effect, water behaves as a non-interfering "window" into the intense Raman spectroscopy of organic compounds dissolved therein. There have been a number of previous reports of Raman spectroscopy in supercritical water but these mostly involve inorganic ions such as metal halides and nitrates. In this laboratory we have developed a simple method to use fiber optic Raman spectroscopy to obtain spectra of organic compounds dissolved in supercritical water. Our objectives were to develop a real-time chemical kinetic probe in order to obtain kinetic and thermodynamic information spectroscopically. As a test system we investigated the hydration of acetic anhydride in supercritical water. We were able to extract several physically relevant constants regarding the decomposition of acetic anhydride under supercritical conditions. Calculations derived from the Raman spectra provided a ΔH value of 70±3 kJ/mol and activation energy of 118± 4 kJ/mol. This is the first physical proof that acetic acid, a weak acid under normal conditions, undergoes almost complete dissociation and behaves as a strong acid under supercritical conditions. This opens additional research opportunities to examine the utility of weak acids to perform acid catalysis under supercritical conditions. Additional acids will also be investigated to build a basis for physical constants under supercritical conditions.

Our current reactor design involves a sealed assembly in which the reactants and solvent are sealed in a cold reactor which is then placed in an oven and heated to attain the conditions necessary to reach the supercritical phase. Because of this design many of our reactions are often monitored at a sub-supercritical state due to the reaction kinetics in a heated environment. In order to overcome this problem an injection system has been designed and the prototype is assembled in our laboratory. Initial tests have begun but there are no current results to report. This assembly will allow reactants to be injected directly into a supercritical environment so that true supercritical water reactions can be monitored.

Samuel Brown
Department of Chemistry and Biochemistry
University of South Carolina
Dissertation Advisor: S. M. Angel
Research Area: Fiber-Optic Sensors

Two types of fiber-optic Raman vapor sensors for enhanced detection of hazardous gases are under development. One design incorporates a previously-described multipass optical cavity. The optical cavity is formed by two spherical or ellipsoidal mirrors aligned with a common focus. A focused laser beam is introduced into the cavity in such a way that it is trapped and reflects repeatedly between the two mirrors. On each reflection, ~100, the laser is refocused, and the Raman scattered light is collected conventionally. In this way enhanced Raman signals can be generated of gases contained in the cell. Recently such a cavity was built for remote operation using optical fibers to deliver the laser and collect the Raman scattered light. Preliminary data with unoptimized cell mirrors show gains of about 10. The performance of this device and suggested improvements will be presented. Also, the potential for miniaturization of this device will be discussed as well as the feasibility of using it to detect solvent vapors in soil and H_2 in tanks.

The other system is designed specifically to be used with a cone penetrometer for identifying solvent vapors in soils from dense nonaqueous-phase liquids (DNAPLs). We have found that a small two-stage thermoelectric- (TE) cooler can be used to "freeze out" many common organic solvent vapors (e.g., CCl_4, tetrachloroethylene/PCE, etc.). The apparatus consists of a two-stage TE cooler mounted on a small aluminum heat sink. A small diamond is mounted on the TE cooler so that it is exposed to the sample vapors which are delivered through a capillary tube directly to the top of the diamond surface. With a two-stage cooler the diamond is cooled to temperatures below -35°. Raman measurements are made of the condensed vapors using a conventional fiber-optic Raman probe that is mounted just above the diamond. The strong diamond Raman band at 1332 cm^{-1} is also used as an internal reference.

A measurement is made with this system by first purging with dry nitrogen to establish a reference baseline. Solvent vapor is then introduced and Raman spectra are measured as the vapor condenses and freezes on the diamond. For CCl_4 and PCE vapors Raman signal intensities typically reach a high value about three minutes after introducing the solvent vapor. We are also investigating the possibility of quantifying the vapor-phase concentration by measuring the rates of adsorption and desorption of the solvent vapor on the diamond heat sink.

Phillip Levine
Department of Geology and Marine Science
University of South Carolina
Dissertation Advisor: C. G. St. C. Kendall
Research Area: Sediment Computer Modeling

As a member of the Stratigraphic Modeling Group of the Departments of Geological Sciences and Computer Science, Mr. Levine's research involved the design and development of the software program SEDPAK. He has been building a forward sedimentary simulation which enables geologists to develop and test sequence stratigraphic models as they visualize their seismic and well data. Sequence stratigraphy is a methodology which is widely used by oil companies in the exploration and exploitation of hydrocarbons.

SEDPAK provides a conceptual framework for modeling the sedimentary fill of basins by visualizing stratal geometries as they are produced between sequence boundaries. The simulation is used to substantiate inferences drawn about the potential for hydrocarbon entrapment and accumulation within a basin. It is designed to model and reconstruct clastic and carbonate sediment geometries which are produced as a response to changing rates of tectonic movement, eustasy, and sedimentation. The simulation enables the evolution of the sedimentary fill of a basin to be tracked, defines the chronostratigraphic framework for the deposition of these sediments, and illustrates the relationship between sequences and systems tracts seen in cores, outcrop, and well and seismic data.

Christopher J. Murray
Department of Geology and Marine Science
University of South Carolina
Dissertation Advisor: Robert Ehrlich
Research Area: Groundwater Geochemical Data Analyses

NMR is a method of gaining information about porosity by quantifying the interactions of atoms and their environment. A degree of success has been achieved involving the relationship between NMR derived pore types and pore types derived from image analysis procedures. Bowers (1992) illustrated that pore size frequency distributions derived from NMR longitudinal relaxation (T_1) experiments are polymodal, indicating the existence of a sub-population of pores. End-members derived from NMR are differentiated by their T_1 relaxation spectral characteristics which are related to pore size and shape. The T_1 values associated with the NMR values are related to the size of pore types determined from image analysis with a constant of proportionality represented by the surface relativity ρ. Surface relaxivity is a measure of the pore wall composition and micro-geometry and scales the NMR response to size. As can be seen, ρ is different for each rock suite thereby complicating our understanding of the controls on ρ and the magnitude of their effect on determining pore size. Presently we do not have a large enough database to adequately quantify ρ. This is especially true for carbonates. A major advantage of the NMR procedure is that it is capable of resolving much smaller pore types than image analysis. Furthermore, NMR pore type data can be coupled with mercury porosimetry data to obtain a complete measure of the pore system. This coupling provides insight into the physical relevance of micropores to formation factor and diffusivity as well as the properties associated with single and multi-phase flow. Mr. Murray's current research is investigating the relationship between NMR pore types and image analysis based pore types using T_2 relaxation times. T_2 is a measure which characterizes the interactions between individual nuclei rather than between the nuclei and the pore wall. Another aspect of the research focuses on the relationship between T_2 and surface relaxivity. Since little work has been done involving T_2 there is no understanding of its relation to ρ. The samples from which thin sections and capillary pressure information are derived are from the Conoco borehole test facility. Nuclear magnetic resonance data, namely T_2 distributions, are being supplied by Conoco in Ponca City, Oklahoma. The thin sections provide a database allowing us to compare image analysis derived pore types with NMR derived pore types using T_2 relaxation times. Capillary pressure information will be used to relate the T_2 data to the multi-phase fluid flow properties of the rocks. Progress thus far has included the determination of image analysis pore types from the original 60 thin sections as well as pore types from an additional set of 22 carbonate thin sections. Mercury injection tests have been run and capillary pressure curves have been obtained for the 25 samples. Progress has also included the analysis of relationships between petrophysical rock properties (porosity, permeability) and properties derived from NMR tests (T_2 information, NMR derived porosity, etc.).

Ray Stewart Williams
Department of Biological Sciences
University of South Carolina
Dissertation Advisor: David E. Lincoln
Research Area: Rising CO_2 Effects on Plant/Insect Interactions

In October of 1993 an experiment was carried out in the Duke University Forest at the site of a long-term study on the effects of elevated CO_2 concentrations on the physiological responses of a major southeastern forest tree species, Loblolly Pine (Pinus taeda). Funded by DOE and EPRI, this project provided Mr. Williams with an excellent opportunity to examine the effects of CO_2 plant growth conditions on the performance of a significant folivore of this tree species, Red-headed Pine Sawfly, (Neodiprion lecontei). The experimental design involved growing pine seedlings under four CO_2 treatments: (1) NC (non-chambered ambient) (2) AMB (chambered ambient) (3) +150 (150 $\mu l\ l^{-1}$ CO_2 above ambient) and (4) +300 (300 $\mu l\ l^{-1}$ CO_2 above ambient). Insects were enclosed on branches of Loblolly Pine for the entire larval life cycle to address the following questions: (1) will elevated CO_2 grown pine seedlings affect the developmental rate and fecundity (measured as male and female pupal weights) of N. Lecontei? (2) will levels of growth or consumption of the larvae differ between treatments? and (3) are alterations in leaf nutritional and defensive chemical constituents responsible for insect responses? Briefly, insects were placed on individual branches (10 per bag) as early instar larvae. On a weekly basis insects were removed, counted to assess mortality, weighed, and returned to the same branches. This procedure was repeated until all insects had reached pupation. At this time, pupae were sexed and weighed to determine fecundity. This experiment was the first time an insect species had been reared throughout its life cycle under field conditions in a global change scenario. Results are not complete but preliminary data analysis suggest that the insects could compensate over the larval life cycle to declining leaf nitrogen contents, resulting in no differences in time to pupation or pupal weights among the treatments. Much of the work Mr. Williams has conducted this year has involved the analysis of leaf phytochemical responses to the CO_2 growth conditions, and statistical analysis of insect performance parameters. Leaves have been analyzed for Kjeldahl nitrogen and monoterpenes, with the quantification of leaf non-structural carbohydrates in progress. When the analysis of all leaf constituents is completed, the information will be related to insect growth and consumption responses. This experiment, as well as the others Mr. Williams has completed, are also in manuscript preparation at this time. The information generated by his research under his EPSCoR fellowship has made a significant contribution to aspects of global climate change research involving trophic level interactions.

James B. Robb II
University of South Carolina
Department of Chemistry and Biochemistry
Dissertation Advisor: James R. Durig
Research Area: Molecular Structures of Organophosphorous Compounds

In the past decade, there has been a substantial increase in the laws, regulations, and uses of environmentally hazardous materials. Phosphorous containing compounds such as pesticides and herbicides as well as chemical warfare agents are of particular interest in the areas of storage, disposal, and treatment of these materials. The need to develop and improve methods to transform these chemicals either stoichiometrically or catalytically into less harmful substances is of great importance. Current research focuses on the analysis of the structural and surface chemistry during the degradation processes. The assignment and characterization of the products are assessed by comparing FTIR spectra to pure reference data. The aspect of the research currently in progress pertains to the conformational stabilities and vibrational assignments of some organophosphorous compounds obtained from Raman and infrared spectra with the aid of *ab initio* calculations. The elucidation of molecular conformational stabilities and the assignment and identification of characteristic functional groups within these compounds will further the ability to develop and improve new methods of treatment and disposal of environmentally hazardous materials by aiding in the determination of the degradation products as well as the surface binding properties of these materials. Additionally, the structural information obtained could be extended to the analysis of larger compounds and provide insight for understanding chemical reaction mechanisms. The focus of the research has been on the following molecules; methoxy dichlorophosphine (CH_3OPCl_2), methoxy difluorophosphine (CH_3OPF_2), ethyl dichlorophosphine ($CH_3CH_2PCl_2$), ethylphosphonic dichloride ($CH_3CH_2P(O)Cl_2$) and chloromethyl difluorophosphine ($ClCH_2PF_2$). For this series of molecules, the structures and conformational stabilities are being investigated relative to the changes of the functional groups attached to the phosphorous atom. The manuscript for methoxy dichlorophosphine has been accepted for publication in the Journal of Molecular Structure and the paper on methoxy difluorophosphine has been completed and is being prepared for review for publication. Nearly all experimental and theoretical work has been completed on the ethyl dichlorophosphine and ethylphosphonic dichloride molecules and manuscripts have been partially written on both molecules where all of the tables have been compiled and the spectral data prepared for publication. The theoretical results on the chloromethyl difluorophosphine molecule are complete and a manuscript has been partially written and all tables and graphs have been compiled for publication.

Edward M. Stack
Department of Geological Science
University of South Carolina
Dissertation Advisor: Dr. Arthur D. Cohen
Research Area: Environmental Geology

We believe that peats have significant potential to be used at DOE sites as sorbents in a variety of waste remediation technologies (e.g. permeable barriers, filters, slurries, etc.). However, our previous research also indicates that peats of different type will have different extraction potentials for different contaminants or combinations of contaminants. Thus, the primary purpose of this research is to determine these differences in sorption capacity for several common contaminants, including dissolved hydrocarbons, metals, and nitrates. A secondary objective is to learn more about the chemical and physical mechanisms by which these hazardous substances are extracted by the peats, with the ultimate goal being either to improve our ability to select the best peat for a specific application or to alter the peat in such a way as to improve its extraction capacity. The tasks involved in accomplishing these goals can be divided into three general categories: (1) hydrocarbon extraction tests; (2) nitrate extraction tests; and (3) metals extraction tests. All of these tests are being run using a wide variety of different peats from the USC Peat Sample Bank. All tests also involve not only different peats but also different concentrations and combinations of contaminants. Depending upon the test, analytical procedures utilized will include, atomic absorption, XRD, microprobe, GC/FT-IR/FID, and pyrolysis GC/MS. The hydrocarbon studies involve slurry tests of the contaminants most often measured at gasoline-contaminated sites, benzene, toluene, ethylbenzene, and xylene (BTEX's). Tests are being run using saturated solutions (in water) of single BTEX's and also of benzene (the most difficult to extract) at three different concentrations (saturated solution, 498 ppm, and 303 ppm). Tests are also being run using saturated solutions of whole gasoline (EXXON Reg, 87 OCT) and peats that are radiated at 1,2,4.5 and 6 megarads to kill any microorganisms. These samples were then tested as is and treated with oxygen, nitrogen and bacteria (Bacillus, Pseudomonas and clostridium). The nitrate extraction studies involve various slurry tests using standard nitrate solutions and different peat types (natural and predried). Laboratory experiments on metals involved 4-5 different peat types and several different metals (cadmium, chromium, zinc, lead, copper, and nickel). These studies consisted of single and multi-component batch-slurry experiments under changing conditions (i.e. temperature, pH, contaminant concentration, etc.). Adsorption-desorption studies of zinc and copper were also carried out on four distinct peat types. Additionally, tests were run at Argonne National Laboratory to determine the potential to separate the different peats into their pure maceral components. This involves use of the density gradient centrifugation procedure developed at Argonne Lab. If this separation can be achieved, the resulting pure components will then be tested at a later date for their chemistries and their extraction capacities. These tests are very significant in that they can lead to a better understanding of peat chemistry (and therefore coal development) and also to a much better understanding of the chemical and physical extraction mechanisms.

Geralyne Lopez-de-Victoria
Department of Biological Sciences
University of South Carolina
Dissertation Advisor: Charles R. Lovell
Research Area: Bioremediation

Bioremediation, or use of microbial transformation of chemical compounds, has proven to be a cost effective solution to the removal of toxic contaminants from wastes sites. For in situ bioremediation to be successful, the microorganisms must survive and proliferate in the areas targeted for cleanup. One of the characteristics influencing bacterial survival and distribution in contaminated environments is their ability to move to (motility), detect (chemotaxis), and use these contaminants. Manipulation of these abilities to our advantage can minimize, and potentially eliminate, the use of disruptive procedures currently being used to achieve mechanical movement of microorganisms in sediments.

In this investigation, Azospirillum, is an excellent model for the study of bacterial motility and chemotaxis to chemical compounds in sediments. Azospirillum , are highly motile nitrogen fixing bacteria commonly found in soils. In the first stages of this investigation, the trainee studied the ability of Azospirillum species to fix nitrogen and use aromatic compounds as carbon sources (Chen et al., 1993). Some of these aromatic compounds, like benzoate and 4-hydroxybenzoic acid, are abundant in contaminated soils. Azospirillum was able to use even toluene, a common contaminant. The trainee also investigated whether Azospirillum can detect these potential nutrient sources and orient their migration towards where they are found. One of the hypotheses was that these aromatic compounds are chemical cues for Azospirillum. Results showed that Azospirillum is chemotactic to these substrates, and more interestingly, that Azospirillum detects them at much lower levels than other soil bacteria (Lopez-de-Victoria and Lovell, 1993). In addition, concentrations at which maximum chemotaxis is observed (peak concentration) and the lowest concentration to elicit a significant response (threshold concentration) were determined for the compounds. After establishing the ability of Azospirillum to use and detect aromatic acids, the motility mechanism by which these organisms move and mediate chemotaxis was examined. Using computer-assisted motion analysis and video microscopy of the three major components of Azospirillum motility were studied (Lopez-de-Victoria and Lovell, 1994). Swimming speed, rate of change in direction (RCDI) and net to gross displacement ratio (NGDR) were determined for the aromatic compounds. Results showed that chemotaxis to aromatic acids was accomplished by a significant increase in swimming speed and NGDR (path linearity) and a decrease in the RCDI (tumbling frequency). Basic understanding of motility and chemotaxis mechanisms is very important in establishing suitable conditions for efficient bioremediation processes. How an organism responds to a chemical and at which concentrations is their movement optimum is critical when designing biodegradation processes. The binding proteins of some of these aromatics and their role in chemoreception is also being investigated.

Derek Sanders
Department of Computer Science
University of South Carolina
Dissertation Advisor: R. L. Cannon
Research Area: Sediment Computer Modeling

Mr. Sanders is currently working on the continuing development and support of SEDPAK. SEDPAK is a suite of applications to be used by exploratory petroleum geologists to forward model the sedimentary filling of basins. This provides the geologist a greater understanding of what processes have affected the basin throughout time and a deeper familiarity with how the basin looks today. This information is then used by the geologists to determine optimal spots for petroleum drilling.

The current development of this program involves several new portions of functionality. New modes of data display have been added, i.e., the user can now look at the kinetic model of maturity present in the current basin. Better control over the current execution display has been implemented. The user can individually pick modes to display within the same window and has interactive control over certain characteristics of those modes, such as which maturity model is being used. A separate program which edits the data filed used by the simulation, and which is included in the package, has also had some new development. Grater flexibility has been given to the user in the manipulation of arrays of data values. For example, the creation of vast arrays has been simplified with a new range creation dialog.

The support of SEDPAK is the most involved activity. This involves finding and correcting bugs reported by geologists who use the program or by the developers themselves. In a project of this magnitude, debugging could be a full-time occupation. Support also involved the refinement of current functionality. As geologists use the program, much is learned about what portions of the interface are too confusing or cryptic, do not provide enough information, or provide information that is different from that expected. Much is also learned about how the data should interact and be displayed upon execution. This is a continually evolving area, and much time has been spent transforming SEDPAK into an easier to use, more intuitive suite of applications.

Istvan Csato
Department of Geology and Marine Science
University of South Carolina
Dissertation Advisor: C. G. St. Kendall
Research Area: Sediment Computer Modeling

Research performed by Mr. Csato includes sequence stratigraphic interpretations and stratigraphic modeling using the program SEDPAK to provide insight into the sedimentary geometries of lacustrine rift basins in the southern Dead Sea and the Pannonian Basin, Hungary.

The research established that in the Dead Sea, nine third-order sequence boundaries can be recognized. Stratigraphic modeling shows that either: lake level falls were delayed by 0.2-0.4 Ma relative to eustatic falls; or lake level changes matched the eustasy, but subsidence rates varied during the basin evolution. The seismic interpretation illustrated that fan-delta sediments accumulated at the two ends of the Dead Sea graben and lacustrine clastics filled the basin. In the northern part of the basin, interfingering of sediments from the southern and northern ends was related to lake level changes. Lake level falls caused transportation of sediment from the northern source, whereas lake level highstrands increased transport of sediments from the south.

In the Pannonian Basin, subsidence ceased in the latest Miocene (Messinian) in the northeastern portion of the Basin, while adjacent blocks continues to subside at high rates. The resulting differential subsidence play an important role in the formation of stratigraphic patterns. Coeval with this tectonic event, a significant lake level fall occurred that produced a basinwide unconformity. Two major deltaic systems filled the northern Pannonian Basin during the Upper Miocene, originating from the northwest and the northeast. Following the Messinian events, the northwestern system remained dominant and filled the rest of the basin.

Stratigraphic modeling revealed that Type 1 and Typed 2 unconformities, and conformity surfaces may develop simultaneously along a basin margin, depending on local subsidence rate. Variations in the amount of sediment supply produced backstepping and progradational patterns, depending on the timing of the change. Encroaching deltas can form various architectural patterns. Lowstand balanced/overwhelming and highstand balanced/overwhelming systems tracts have been proposed as end-members for the interfingering configurations.

Sean R. Ryan
Department of Geology and Marine Science
University of South Carolina
Dissertation Advisor: C. G. St. Kendall
Research Area: Stratigraphic Modeling

Research performed for January 1995 to May 1995

Mr. Ryan's research has involved the modeling of the sequence stratigraphy of the National Petroleum Reserve of Alaska. He has established that the Nanushuk formation consists of the proximal sandier facies of the Torok formation prograding complex. The depositional sequence framework for the Torok and Nanushuk formations, established using regional seismic and well data, reveals an eastward prograding shelf edge which is bounded by a series of type 1 unconformities. High amplitude 3rd order eustatic events are superimposed on the longer term events of relative sea level changes. These eustatic events (major sea level falls followed by second order rises) created characteristic geometric patterns of the depositional margin, including packages of sigmoidal reflectors and downlapping lowstand systems tracts. These depositional geometries were simulated in order to determine the relationship between the sequenced and the variables which affect relative sea level (sea level position, clastic supply, and subsidence). Modeling these packages: 1) confirmed the existence of major 2nd and 3rd order eustatic sea level variation in the Aptian/Albian; 2) demonstrated that these major eustatic changes were the primary control for the development of the stratal geometries within the Torok and Nanushuk formations; and 3) provided a framework to address reservoir distribution and potential migration pathways within these formations. Additionally Mr. Ryan has been testing the development of SEDPAK.

C. PRACTICUM/COLLABORATION EXPERIENCES

Bradley Johnson

All activities described in part B were performed in collaboration with Hoechst Celeanese Corporation under the supervision of Dr. Robert Sportnitz (704-587-8537). Hoechst Celanese benefited directly by the construction of the electrochemical apparatus. As Hoechst Celanese is the world's leading producer of battery separators for the lithium ion battery, they have an interest in developing a system by which their separators could be tested under a realistic environment. The development of a lithium ion battery model will be important to Hoechst Celanese as they will be able to determine the most important separator parameters which affect lithium ion bettery performance

Christopher Bunker

None reported at date of report.

Steven Christopher

A two day trip to the sole manufacturer of charge injection devices, CID Technologies, Liverpool, NY was organized by David Carta (CIDTEC) and Dr. R. Kenneth Marcus (Clemson University). The purpose of the trip was for Mr. Christopher to become more familiar with the electrical operation of the CID imagers and to learn the procedure for changing/replacing the imagers on the CID remote head. Emphasis was placed on CID sources of noise, and the different readout and data collection modes of the device.

Patrick Joyce

None reported at date of report.

Scott Brame

Condensed and edited a thesis by David Kroening that dealt with rehabilitation of wells clogged at the Westinghouse Savannah River Site. The final form of the paper was accepted for publication by the journal *Groundwater Monitoring and Remediation* this spring or summer.

Stewart Edmunds

The studies were conducted in collaboration with the NOAA Southeast Fisheries Science Laboratory in Chareston. The work was conducted at this NOAA facility and reported to laboratory officials on a regular basis. The contact scientist at the laboratory is Dr. Sylvia Galloway, Laboratory Director (803) 762-8617. The benefits received by NOAA was the development of a methodology that is needed by its Ecotoxicology Program for conducting studies an the effects of agriculture pesticide run-off in South Carolina and Florida. This work is also providing a means to aid the aquaculture industry, specifically examining feed for estrogenic activity. Finfish are very sensitive to

estrogenic substances and these agents can substantially decrease somatic productivity. The benefits received by the student was direct supervision of the research project by laboratory scientists in the Ecotoxicology, Marine Toxins and Marine Biotechnology Programs. Substantial interaction was also found from staff in the adjoining laboratories which were examining the field samples for contaminants using analytical and assay procedures.

Albrecht Carver

None reported at date of report

James Roane

This project is a collaborative effort among Clemson University, Rust Federal Services' Clemson Technical Center, and Bradtec-GB, Inc. All of the work performed to date has been a joint effort of Clemson University and Rust. The practicum contact is Dr. John Leyba (864-646-2413). The benefits for Rust are those that accrue from active participation in the development of instrumentation that offers the promise of decreasing the time and labor required to perform radiological analyses of samples. Though their involvement at this stage of the effort, they have the opportunity to evaluate its benefits, recognize its limitations, and provide suggestions for improvements. The benefits to the student include an exposure to the industrial perspective, the availability of resources beyond those that the University can provide, and the early cultivation of industrial contacts.

Shawn White

Research on this project was conducted in collaboration with the Westinghouse Savannah River Site in Aiken, South Carolina, via a SCUREF Task Order #151.
Contact: Dr. Pat O'Rourke (803-725-2173).

Wendy Bell

This project was begun with the initial goal of development of useful organic reactions in supercritical water, leading to the replacement of conventional organic reactions in supercritical water, and thereby reducing pollution at its source. This work began as a collaborative effort between the laboratories of Edith Parsons and Joe Kolis at Clemson University and Michael Myrick at the University of South Carolina. Guidance has been provided by Mike Cushman at Eastman Chemical Company to insure the applicability of the work to real-world industrial situations. The student has gained insight into how to formulate proposed fundamental research to have direct applicability to the industrial community.
Contact: Mike Cushman
Head, Environmental Research Laboratory
Eastman Chemical Company
(615) 229-4075

Samuel Brown

Mr. Brown is working with LLNL to develop improved methods of detecting environmental contaminants in-situ. He is currently working on sensors for uranyl, and perchloroethylene. LLNL benefits from this arrangement by obtaining technical information on new ways to measure these analytes. USC and the student benefit by LLNL expertise in optical engineering and by equipment supplied by LLNL for some of the research.
Contact: Dr. Fred Milanovich, Lawrence Livermore National Laboratory (LLNL), (510) 422-6838

Mr. Brown is working with NOSC to develop Raman sensors for measuring solvent soil contaminants (DNAPLs). NOSC will have access to the techniques developed. USC and the student will benefit from NOSCs expertise in groundwater measurements and by supplies contributed by NOSC to the project.
Contact: Dr. Stephen Lieberman, Naval Ocean Center (NOSC). (619) 553-2778

Phillip Levine

Mr. Levine taught a three day short course for Amoco Production Company entitled "Stratigraphic simulation: a new exploration/exploitation". The course was attended by employees of Amoco, Texaco, and Conoco.

Together with Derek Sanders and Istvan Csato, Mr. Levine developed two thermal maturation models within SEDPAK. These include the Lopatin-Waples TTI (time temperature index) model (Waples, 1980) and the Arrhenius equation kinetic model (Tissot et al., 1987). This work involved a number of oil companies including Amoco, Conoco, Texaco and Petrobras.

In addition, major studies involving SEDPAK were conducted at Texaco and Amoco.
Contact: Dr. Susan Nissen, Amoco Production Company, Research Center
(918) 660-3518

Christopher Murray

The practicum was done under the aegis of the Savannah River Technology Center during the period of June 1993 to September 1993. The practicum focused on the Burial Ground site in the General Separations Area. Data used in the study was in the form of water geochemistry data for the three aquifers in the project sites. These aquifers, in order of depth, are known as the water table aquifer, the Bamwell/McBean aquifer, and the Congaree aquifer. The geochemical data was analyzed using polytopic vector analysis, an unmixing algorithm which determines the number of end members in a data matrix, the chemical compositions of the end members, and the compositions of the samples in terms of the end members. This procedure allows for the determination of the number of sources of contamination, the chemical compositions of these sources, and to model the flow of these contaminants based on the proportion of these end members in the samples at each sampling site. Two problems with the data

had to be overcome. The first problem was that the geochemical data on diskettes was not in the correct format to be analyzed using our in house multivariate analysis procedures. The only recourse was to type the data in by hand in the correct format, a lengthy procedure. Secondly, much of the data was unusable because the concentrations of many of the contaminants were below detection limits. Hence, only a small percentage of the contaminants tested for were included in the study. Separate analyses were run for each of the three aquifers, with each aquifer having its own set of end members and sample compositions. Most of the end members for all aquifers were dominated by one contaminant that comprised over 60% of that end member. Initial results showed that many of the end members occurred predominantly in localized areas of the Burial Ground, indicating that samples in these areas were composed mainly of one end member. This data provides information on the sources of contamination. For instance, many of these areas represented by a single end member coincide with the location of a plume leaking out from a burial site, indicating a relationship between an end member and the contaminants in the plume. In some cases these areas dominated by a single end member reflected the geology. An example would be an end member composed mainly of calcite occurring predominantly in an area of limestone terrain. These results provide important information on the movement of contaminants through the groundwater system. Results have also shown that some wells which penetrate all three aquifers have samples that are dominated by end members with different chemical compositions, indicating that contaminant flow is not the same between aquifers. This provides information on how the aquifers are related hydrologically with respect to contaminant flow. Research is continuing. Results of the practicum were presented to the Savannah River Technology Center. In addition, Dr. Robert Ehrlich presented the results at a meeting of the Aiken Geological Society on November 30, 1994.
Contact: Mary Harris (803) 644-6754

Ray Williams

Mr. Williams conducted the practicum at Oak Ridge National Laboratory, Oak Ridge, Tennessee. His experiments at ORNL began in April and were completed (field aspects) in July of 1993. His experience at this national laboratory was rewarding both professionally and personally. A successful and ongoing collaboration was established with Dr. Richard Norby (Environmental Sciences Division,. Telephone: (615) 576-5261). Dr. Norby has made significant contributions to global change research and this collaboration was seen as an important component of his research mission at ORNL. Utilizing White Oak seedlings in a ongoing, long-term experiment, Mr. Williams was able to examine alterations in the performance of significant tree feeding insects (Gypsy Moth, Forest Tent Caterpillar, and Fall Cankerworin) relative to elevated C02 growth conditions. The experiments conducted here contribute to the overall larger objective of global climate change research to examine ecosystem responses such as trophic level interactions.

James Robb

The practicum was conducted at the DOE/Westinghouse Savannah River Site (SRS) in Aiken, SC from 23 May 1994 to 28 August 1994. Research was carried out under the supervision of Henry Randolph, a physicist in the equipment engineering division. The research conducted at the facility was centered around a glassification process for the storage of low level radioactive waste materials and consisted of the design, testing, and calibration of microcapillary gas chromatographs to sample the gases from the current storage tanks and the reaction vessel and determine whether or not the gases present were a possible explosion hazard. This project was in conjunction with several other divisions of the SRS facility and weekly progress reports were presented to other heads of departments in which discussion of the progress towards completion of the project was assessed. Besides gaining experience in the programming, design, testing, and sampling techniques of gas chromatography, valuable experience was obtained by observing how the government and a large corporation operate through communication and also the procedures that must be followed throughout every aspect of the project. Also, monthly meetings and training sessions covering various safety procedures were required which provided valuable instructions on how the corporate system works to attain a safe working environment. Additionally, the trainee was able to work on other areas of the glassification project as well as on different research and development projects in which the trainee's ideas and contributions to these efforts were helpful in the advancement of the research.
Contact: Henry Randolph, (803) 725-1245

Edward M. Stack

The practicum experience took place at Argonne National Laboratory between June 1 and December 1, 1992 and October 8 and December 15, 1993 under the technical supervision of Dr. Gary Dyrkacz, Chemistry Division (708-252-7478). It involved continuation of an earlier attempt to develop a gradient medium that would allow density-gradient separation of peats into their maceral components. Dr. Dyrkacz is one of the innovators of this technique and the instrumentation at Argonne Lab is, consequently, state-of-the-art. Dyrkacz has successfully separated ground coals into their maceral components; but, prior to this study, this technique had never been tried on peats. The studies were conducted on 15 peat types. The initial studies used calcium nitrate, sodium chloride or cesium chloride as media along with varying concentrations of 30 different surfactants. The results showed aggregation of the organics and poor density reading. The study was then shifted to the use of an organic gradient of tetrabromoethane using polyvinylpyrrolidone-40 as a surfactant. This medium produced a break-through in that several peats now showed very promising results for maceral separation. Continuous flow separation was then conducted and 56 separate samples produced by this method were collected between 1.4 and 1.7 density and analyzed with FT-IR at Argonne Lab. Pellets samples embedded in expoxy are being studied at USC for reflectance. Also, Patrick Hatcher, a leading fuel chemist at Pennsylvania State University, has been analyzing samples using pyrolysis GC-MS.

Geralyne Lopez-de-Victoria

The three-month practicum was to be performed from May-July, 1995, at the Savannah River Laboratory in Aiken, SC under the supervision of Dr. Terry C. Hazen. Dr. Hazen has been involved for several years with the DOE Subsurface and bioremediation programs at SRP. The trainee did not perform the scheduled practicum due to an unexpected pregnancy. Ms. Lopez-de-Victoria has been awarded a Postdoctoral Fellowship at the SRP at the writing of this report.
Contact: Dr. Terry C. Hazen, (803) 725 7517

Derek Sanders

SEDPAK is currently being used by several major petroleum companies. As a developer, Mr. Sanders discusses the ramifications and merits of additions or changes to the current program with representatives from these companies at periodic meetings. He also assists those members who are having problems with installation or getting started with the program.
Contact: T.L. Burnett, Texaco, (713) 432-6808

Istvan Csato

Together with Derek Sanders and Phillip Levine, Mr. Csato was involved with the development of different thermal maturation models for SEDPAK. These include the Lopatin-Waples TTI (time temperature index) model (Waples, 1980) and the Arrhenius equation kinetic model (Tissot et. al., 1987). This work involved a number of oil companies including Amoco, Conoco, Texaco, and Petrobras.
Contact: Dr. Garry Proddy, Texaco, Research Center, (713-954-6018).

Sean Ryan

Mr. Ryan has developed a liason with the Petroleum Division of the Alaskan Survey to retrieve seismic data. He has produced a home page to inform the oil industry of the research activities we are performing. He has constructed exercises to teach the oil industry how to use the SEDPAK program.
Contact: Dr. Tim Ryherd, Alaskan Division of Oil and Gas, (907) 762-2140.

D. SELECTED DEVELOPMENTS

Bradley Johnson

Although no publications have emerged from this work, it is expected that as soon as the model is developed, joint publications will emerge.

Christopher Bunker

Bunker, C.E., Ma, B., Ma, J.J., DesMarteau, D.D., Sun, Y.-P., "Steady-State and Time-Resolved Studies of Fluorescent Molecular Probes in Nafion Films" (in preparation)

Steven Christopher

Oral Presentation: "The Direct Imaging of Ions Using a Charge Injection Device Detector" at the 1995 Pittsburgh Conference, New Orleans Convention Center, New Orleans, LA.
Poster Presentation: "The Direct Imaging of Ions Using a Charge Injection Device Detector" at the 1995 American Society for Mass Spectrometry (ASMS) Conference in Atlanta GA.
Oral Presentation: "The Direct Imaging of Radio Frequency Glow Discharge Ions", doctoral candidate student seminar requirement, Department of Chemistry, Clemson University, Clemson, SC.

Patrick Joyce

None reported at date of report.

Scott Brame

None reported at date of report.

Stewart Edmunds

Mr. Edmunds presented the assay methodology at the XIII International Neurotoxicology Conference Series (October 29 - November 1, 1995). The conference theme was Developmental Neurotoxicity of Endocrine Disrupters: Dioxins, PCBs, Metals, Pesticides, Psychoactive and Theraputic Drugs and had over 200 participants from industry, government, and universities representing 17 countries. The paper was entered in the student competition and evaluated for significance, quality of work, presentation, and knowledge of subject. Mr. Edmunds was awarded the Second Place Award and received a certificate and a small cash award. The work was invited for publication by the Editor-in-Chief of Neurotoxicology, Dr. Joan Cranmer and is currently under peer review by the journal. The manuscript is entitled "Development of a Rapid and Sensitive High Throughput Reporter Gene Assay for Estrogenic Contaminants".

Albrecht Carver

Paper: "Image Processing Algorithm Design and Implementation for Real-Time Autonomous Inspection of Mixed Waste", was accepted for the SPIE Visual Communications and Image Processing '96 Conference to be held 17-20 March 1996 in Orlando, Florida.

James Roane

Fjeld, R. A., DeVol, T. A., Leyba, J. D. and Roane, J. E. "Measurement of Radionuclides Using Ion Chromatography and Flow-Cell Scintillation Counting with Pulse Shape Discrimination for ER/WM Applications", presented at Environmental Technology Development through Industry Partnership, Morgantown WV, October 3 - 5, 1995.

Shawn White

None reported at date of report.

Wendy Bell

Developments resulting from this research include a patent which has been filed titled, "Fiber Optic In-Situ Probe for Monitoring High Pressure, High Temperature Reactions". A manuscript entitled "Real-Time Determination of Chemical Kinetics via In-Situ Raman Spectroscopy in a Hydrothermal/Supercritical Water Reactor" is due to be submitted for publication to Applied Spectroscopy in early 1996. In addition, three presentations have been made on the results obtained from the research activity during the report period. These include:

"Hydrolysis of an Anhydride in a Hydrothermal/Supercritical Water Reactor: A Raman/Chemometric Study of Real-Time Chemical Kinetics", W.C. Bell, G.A. Loungeway, K.S. Booksh, T.A. Bryson, and M.L. Myrick, Eastern Analytical Symposium, Sommerset, NJ, Novermber 13-15, 1995.

"In-Situ Optical Studies of Chemical Reactions in Supercritical Water", W.C. Bell, M.L. Myrick, K.S. Booksh, T.A. Bryson, G.A. Loungeway, ACS Regional Meeting, Memphis, TN, November 28 - December 1, 1995.

"In-Situ Raman Spectroscopy in a Hydrothermal/Supercritical Water Reactor: Real-Time Determination of Chemical Kinetics", W.C. Bell, K.S. Booksh, M.L. Myrick, PitCon 96, Chicago, IL, March 3-8, 1996.

Samuel Brown

The TE-cooled Raman cell may be patentable. We are also extending this work with NOSC to include TE-cooled surface-enhanced Raman sensors which also might be patentable.

Phillip Levine

For the present report period:

Instructor for two day American Association of Petroleum Geologists short course, Sequence stratigraphic simulation: a new tool for exploration/ production.

R.E. Prueser, P.A. Levine, G.R. Baum, and C.G.St.C. Kendall, Sequence stratigraphy and stratigraphic simulation of the Brent Group, Norwegian North Sea (abs.): AAPG Annual Convention Official Program, (submitted).

J. Reistroffer, P.A. Levine, C.G.St.C. Kendall, and A. Finno, Exploration for stratigraphic traps in a foreland basin using a sequence stratigraphic simulation:

examples from the Eocene/Oligocene of the Apure-Llanos Basin, Venezuela (abs.): AAPG Annual Convention Official Program, (submitted).

C.G.St. C Kendall, P.A. Levine, and R. Ehrlich, The enigma of 3rd-order sea level cycles: a cosmic connection? In B.U. Haq, ed., Sequence stratigraphy and depositional response to eustatic, tectonic, and climatic forcing: SEPM Special Publication, (in press).

Christopher Murray

Mr. Murray completed a paper entitled "An Evaluation of the Diagenetic and Structural Influence of Hydrocarbon Entrapment in the Cardium Formation, Deep Basin, Western Alberta". This paper was accepted for publication in the *Bulletin of Canadian Petroleum Geology* and can be found in the December 1994 issue.

Ray Williams

Mr. Williams has conducted several experiments in the area of plant-insect interactions related to global climate change. His dissertation research has involved two successful collaborations with Duke University and Oak Ridge National Laboratory scientists, and has contributed a substantial body of empirical evidence towards our understanding of how increasing atmospheric C02 may alter the interactions between tree species and significant herbivorous consumers of them.

James B. Robb

Mr. Robb's research advisor, Dr. James R. Durig, has been asked to present an invited paper at the International Chemical Congress of the Pacific Basin Societies at their meeting in December in 1995. Much of Mr. Robb's research will be the content of this talk. Professor Durig has also presented several papers on organophosphorous studies at the International Conference on Raman Spectroscopy, the European Conference on Molecular Spectroscopy, the Chemical Society of Canada, the American Chemical Society Midwest Regional Meeting, and the Ohio State Molecular Spectroscopy Symposium. The results on these molecules have been presented to international audiences and will lead to review articles co-authored with the trainee which should be useful for pointing out further studies that are needed for these important environmental compounds.

Edward M. Stack

Mr. Ed Stack has co-authored oral papers at two national conferences on environmental remediation. The two talks were presented at a conferences titled "Emerging Technologies in Hazardous Waste V" held September 27-29, 1993 in Atlanta and sponsored by the Engineering Chemistry Division of the American Chemical Society. The graduate trainee has also co-authored an additional two oral papers at the conference titled "Emerging Technologies in Hazardous Waste VI" held September 19-21, 1994 in Atlanta and sponsored by the Engineering Chemistry Division of the American Chemical Society. Mr. Stack also participated in a workshop in Houston, Texas on May 10-13, 1994 entitled "Hydrocarbon Contaminated Soils and Groundwater" (Second Annual Technical Seminar) sponsored by the Association for

the Environmental Health of Soils. This consisted of technical presentations and evening workshops. The evening workshops included "Soil Remediation Workshops I and II" and "Fundamentals and Applications of Bioremediation to Contaminated Soils".Additional publications during the period included:

Stack, E.M., Eltayeb, S., Liu, J., Cohen, A.D., and Durig, J.R., 1994, The Use of Characterized Peats as Sorption Media for Heavy Metals: Emerging Technologies in Hazardous Waste Management VI, American Chemical Society, pp. 1001.

Stack, E.M., Eltayeb, S., Liu, J., Cohen, A.D., and Durig, J.R., 1994, BTEX Sorption Potential of Natural, Radiated and Bioenhanced Characterized Peats: Emerging Technologies in Hazardous Waste Management VI, American Chemical Society, pp. 1136.

G. Lopez-de-Victoria

During the course of Ms Lopez-de-Victoria's investigation numerous and favorable developments have occurred. At the beginning, she and Professor Lovell were able to document the widely spread ability among soil bacteria to use aromatic compounds. Previously this ability was thought to be found only in a limited number of microorganisms, some of which are not suitable for use in bioremediation. In addition, the chemotaxis experiments demonstrated that Azospirillum spp., the model organism, is able to detect these compounds at nanomolar concentrations, much lower levels than other common soil bacteria like Pseudomonas spp. Most importantly the exact mechanism by which Azospirillum moves to these compounds was established. This was the first time that swimming mechanics of Azospirillum species had been studied. From these experiments they found preferential responses to some aromatics than to others and different chemotactic patterns between the two Azospirillum spp. studied. These results stimulated the trainee's interest in studying in more depth some of the physiology involved in the detection of these aromatic compounds. Important was also the ability to use computer assisted motion analysis for looking at three major components of bacterial behavior in response to chemicals, more precisely than other more time consuming methods.

Derek Sanders

None reported at date of report.

Istvan Csato

1996, Csato I., and C.G.St.C. Kendall, "Sequence Stratigraphic Interpretations in a Continental Strike-Slip basin - Southern Dead Sea, Israel (abs.): AAPG Annual Convention Official Program (submitted)

1995, Csato I., and C.G.St.C. Kendall, "Late Miocene Deltaic Fill of the Pannonian Basin, Hungary: Its Implication to Stratigraphic Architectures and Rervoirs (abs.): AAPG Annual Convention Official Program, p. 20.

Sean Ryan

1996, Ryan, Sean R., Christopher G.St.C. Kendall and Gerald R. Baum, "Depositional Sequence Analysis and Stratigraphic Simulation of the Aptian/Albian Torok and Nanushuk Formations, National Petroleum Reserve, North Slope of Alaska: (in press with the program of the Annual Meeting for the American Association of Petroleum Geologists).

REQUEST FOR ADVANCE OR REIMBURSEMENT	1. TYPE OF PAYMENT REQUESTED		2. BASIS OF REQUEST	
3. FEDERAL SPONSORING AGENCY	( )Advance	(X) Reimbursement	(X) Cash	( ) Accrual
US DEPARTMENT OF ENERGY	4. FEDERAL GRANT NUMBER DEFG0291ER75663		5. PARTIAL PAYMENT REQUEST NUMBER 38	
	7. RECIPIENT'S ACCOUNT NUMBER		8. PERIOD COVERED BY THIS REQUEST	
6. EMPLOYER IDENTIFICATION NUMBER: 576001153	13100P115 & Z108 & Z114		10/1/95	12/31/95

9. RECIPIENT ORGANIZATION	10. PAYEE
University of South Carolina Contract & Grant Accounting 516 1/2 South Main Street Columbia, South Carolina 29208	University of SC - Financial Services Accounts Receivable PO Box 86900 Columbia, South Carolina 29208

11. COMPUTATION OF AMOUNT OF REIMBURSEMENTS/ADVANCES REQUESTED

PROGRAMS/FUNCTIONS/ACTIVITIES >	(a)	(b)	(c)	Total
A. Total Program Outlays to Date	$1,280,083.81	$0.00	$0.00	$1,280,083.81
B. Less: Cumulative Program Income	$0.00	$0.00	$0.00	$0.00
C. Net Program Outlays (Line A. minus Line B.)	$1,280,083.81	$0.00	$0.00	$1,280,083.81
D. Estimated Net Cash Outlays for Advance Period	$0.00	$0.00	$0.00	$0.00
E. Total (Sum of Lines C. and D.)	$1,280,083.81	$0.00	$0.00	$1,280,083.81
F. Non-Federal Share of Amount on Line E.	$530,276.63	$0.00	$0.00	$530,276.63
G. Federal Share of Amount on Line E.	$749,807.18	$0.00	$0.00	$749,807.18
H. Federal Payments Previously Requested	$747,192.64	$0.00	$0.00	$747,192.64
I. Federal Share Now Requested (Line G. Minus Line H.	$2,614.54	$0.00	$0.00	$2,614.54
J. Advanced Required by Month When Requested :1ST MTH	//////////	//////////	//////////	//////////
By Federal Grantor Agency for Use in :2ND MTH	//////////	//////////	//////////	//////////
Making Pre-Scheduled Advances :3RD MTH	//////////	//////////	//////////	//////////

12. Alternate Computation for Advances Only	
A. Estimated Federal cash outlays that will be made during period covered by the advance	$0.00
B. Less: Estimated Balance of Federal Cash on Hand as of beginning of advance period	$0.00
C. Amount Requested (Line A. Minus Line B)	$0.00

13. Certification

"I certify that to the best of my knowledge and belief the data above iscorrect and that all outlays were made in accordance with the grant conditions or other agreement and that payment is due and has not been previously requested.

Signature of Authorized Certifying Official	Date Submitted
Patrick T. Blackwell	05-Apr-96
Typed or Printed Name and Title	Telephone Number
Tony Huggins, Cash Accounting	(803) 777-4850

THIS SPACE FOR AGENCY USE

SF 270 FINAL REQUEST

FEDERAL CASH TRANSACTIONS REPORT AMENDED 4/5/96

1. FEDERAL SPONSORING AGENCY Department of Energy	2. RECIPIENT ORGANIZATION University of South Carolina Contract & Grant Accounting 516 1/2 South Main Street Columbia, South Carolina 29208	
3. FEDERAL EMPLOYER ID NUMBER 576001153	4. FEDERAL GRANT NUMBER DE-FG02-91ER75663	5. RECIPIENT NUMBER 13100 F115
6. LETTER OF CREDIT NUMBER	7. LAST PAYMENT NUMBER 36	8. PAYMENT VOUCHERS CREDITED 36
9. TREASURY CHECKS RECEIVED 36	10. PERIOD COVERED BY THIS REPORT From:	To:
11. STATUS OF FEDERAL CASH	10/1/95	12/31/95
A. Cash on Hand Beginning of Reporting Period		($12,639.61)
B. Letter of Credit Withdrawals		$0.00
C. Treasury Check Payments		$12,636.61
D. Total Receips (Sum of Lines B. and C.)		$12,636.61
E. Total Cash Available (Sum of Lines A. and D.)		($3.00)
F. Gross Disbursements		$61,118.05
G. Federal Share of Program Income		$0.00
H. Net Disbursements (Line F. Minus Line G.)		$61,118.05
I. Adjustments of Prior Periods		
J. Cash on Hand End of Period		($61,121.05)
12. The amount shown on line 11j above, represents cash requirements for the ensuing ( ) days		
13. OTHER INFORMATION		
A. Interest Income		$0.00
B. Advances to Subgrantees or Subcontractors		$0.00
14. REMARKS (Attach Additional Sheets of Plain Paper if more Space is Required)		

15. CERTIFICATION

"I certify to the best of my knowledge and belief that this report is true in all respects and that all disbursements have been made for the purpose and conditions of the grant or agreement."

Signature of Certifying Official Patrick T. Blackwell	Date Report Submitted 05-Apr-96
Typed or Printed Name and Title Patrick T. Blackwell, Associate Director	Telephone (803) 777-4850
THIS SPACE FOR AGENCY USE	

Standard Form 272 AMENDED 4/5/96

AMENDED 4/5/96

FINANCIAL STATUS REPORT
(Short Form)

1. Federal Agency U.S. Department of Energy	2. Federal Grant Number DE-FG02-91ER75663	OMB Approval # 0348-0039	Page 1 of 1

3. Recipient Organization (Name and Complete Address, Including Zip Code)

University of South Carolina
Contract & Grant Accounting
516 1/2 South Main Street
Columbia, South Carolina 29208

4. Employer Identification #	5. Recipient Account Number	6. Final Report	7. Basis
576001153	13100 P115	(X) Yes ( ) No	(X) Cash ( ) Accrual

8. Funding/Grant Period From:(Month, Day, Year)	To:(Month, Day, Year)	9. Period covered by this Report From:(Month, Day, Year)	To:(Month, Day, Year)
9/30/91	12/31/95	10/01/94	12/31/95

10. Transactions:	Previously Reported	This Period	Cumulative
A. TOTAL OUTLAYS	$849,968.16	$436,115.65	$1,286,083.81
B. RECIPIENT SHARE OF OUTLAYS	$288,587.59	$241,689.04	$530,276.63
C. FEDERAL SHARE OF OUTLAYS	$561,380.57	$188,426.61	$749,807.18
D. TOTAL UNLIQUIDATED OBLIGATIONS	**********	**********	$0.00
E. RECIPIENT SHARE OF UNLIQUIDATED OBLIGATIONS	**********	**********	$0.00
F. FEDERAL SHARE OF UNLIQUIDATED OBLIGATIONS	**********	**********	$0.00
G. TOTAL FEDERAL SHARE (SUM OF LINES C AND F)	**********	**********	$749,807.18
H. TOTAL FEDERAL FUNDS AUTHORIZED FOR THIS FUNDING PERIOD	**********	**********	$750,000.00
I. UNOBLIGATED BALANCE OF FEDERAL FUNDS (LINE H MINUS G)	**********	**********	$192.82

11. Indirect Expense	a. Type of Rate (Place "X" in appropriate box) ( ) Provisional	(X) Predetermined	( ) Final	( ) Fixed
	b. Rate N/A	c. Base N/A	d. Total Amount N/A	e. Federal Share N/A

12. Remarks: Attach any explanations deemed necessaryfor information required by Federal sponsoring agency in compliance with governing legislation.

13. Certification: I certify to the best of my knowlege and belief that this report is correct and complete and that all outlays and unliquidated obligations are for the purposes set forthin the award documents.

Typed or Printed Name and Title	Telephone (Area code, number, and ext)
Patrick T. Blackwell, Associate Director	(803)777-4856
Signature of Authorized Certifying Official Patrick T. Blackwell	Date Report Submitted APRIL 5, 1996

SF269A AMENDED 4/5/96

APPENDIX

Vitae of Research Advisors

Ralph E. White
Department of Chemical Engineering
University of South Carolina, Columbia, SC 29208
Telephone: (803) 777-3270
FAX: (803) 777-8265
E-Mail: rew@sun.che.scarolina.edu

Education

Ph.D., 1977, Chemical Engineering, University of California at Berkeley
M.S., 1973, Chemical Engineering, University of California at Berkeley
B.S., 1971, Engineering, University of South Carolina

Professional Employment

Director of the Center for Electrochemical Engineering, 1995-present
Professor, Chemical Engineering, University of South Carolina, 1993-present
Chairman of the Department of Chemical Engineering, University of South Carolina, 1993-present
Distinguished Scientist, Westinghouse Savannah River Company, 1993-present
Associate Head of the Department of Chemical Engineering, Texas A&M University, 1990-1992
Professor, Chemical Engineering, Texas A&M University, 1985-1992
Associate Professor, Chemical Engineering, Texas A&M University, 1981-1985
Assistant Professor, Chemical Engineering, Texas A&M University, 1977-1981

Society Memberships / Professional Honors

American Institute of Chemical Engineers — Phi Beta Kappa
The Electrochemical Society, Treasurer (1990-1994) — Tau Beta Pi
Battery Division Research Award - The Electrochemical Society, Inc., 1991
Electrodeposition Division Research Award - The Electrochemical Society, Inc., 1992
Journal of the American Electroplaters and Surface Finishers Society, Silver Medal Award, 1993

Total Number of Refereed Publications	136
Total Number of Books Edited or Co-Edited	28
Total Contributed Chapters to Books	40

Research Interests

Electrochemical systems, mathematical modeling, batteries, corrosion, electrodeposition

Five Recent Publications

D. H. Coleman, R. E. White and D. T. Hobbs, "A Parallel Plate Electrochemical Reactor (PPER) Model for the Destruction of Nitrate and Nitrite in Alkaline Waste Solutions," *Journal of the Electrochemical Society,* **142** (1995) 1152-1161.

Pauline De Vidts and Ralph E. White, "Mathematical Modeling of a Nickel-Cadmium Cell: Proton Diffusion in the Nickel Electrode," *Journal of the Electrochemical Society,* **142** (1995) 1509-1519.

J. Landfors, D. Simonsson, R. E. White, "Discharge Behavior of Tubular Lead Dioxide Electrodes III. Two-Dimensional Current Density Distribution," *Journal of Applied Electrochemistry,* **25** (1995) 315-325.

B. N. Popov, G. Zheng, and R. E. White, "Electroplating of Thin Films of Bismuth Onto Type 4340 Steel and Alloy 718 to Prevent Hydrogen Embrittlement," *Corrosion Science,* **51,** No. 6, (1995) 429-435.

G. Zheng, B. N. Popov, and R. E. White, "Electrochemical Determination of the Diffusion Coefficient of Hydrogen through a $LaNi_{4.25}Al_{0.75}$ Electrode in Alkaline Aqueous Solution," *Journal of the Electrochemical Society,* **142** (1995) 2695-2698.

Ya-Ping Sun
Department of Chemistry
H. L. Hunter Chemistry Laboratory
Clemson University, Clemson, South Carolina 29634-1905
Telephone: (864) 656-5026
FAX: (864) 656-6613
E-Mail: syaping@clemson.edu

Education

Ph.D., Florida State University, 1989, Chemistry (J. Saltiel, Advisor)
M.S., Zhejiang University, China, 1985, Chemical Thermodynamics (W.-H. Yen, Adviser)
B. Eng., Zhejiang Institute of Technology, China, 1982, Chemical Engineering

Professional Experience

1992-Present, Assistant Professor, Department of Chemistry, Clemson University
1989-1992, Postdoctoral Fellow, Chemistry, University of Texas at Austin (J. Michl, M. A. Fox)

Memberships

American Chemical Society, Inter-American Photochemical Society, American Society of Photobiology

Honors

1988 Graduate Research Award, Florida State University

Teaching Experience

Analytical Chemistry, Organic Chemistry

Collaborators over the past 48 months

Professor K. P. Johnston, University of Texas at Austin
Dr. D. Dabestani, Oak Ridge National Laboratory

Students and Postdoctoral Associates over the past 60 months

C. E. Bunker, T. L. Bowen; G. E. Lawson; B. Ma; P. L. Wickremesinghe; H. W. Rollins; B. Liu; N. B. Hamilton; J. McGown; C. A. Lytle; C. Farmer; R.-Q. Xie

Recent Research Papers (Since 1993)

"Photoinduced Inter- and Intra-Molecular Electron Transfer Reactions of C_{60} and Tertiary Amine. Formation of Cycloadduct N-Ethyl-trans-2',5'-dimethylpyrrolidino[3',4':1,2][60]fullerene

"Evidence for Enhanced Biomolecular Reactions in Supercritical CO_2 at Near-Critical Densities from a Time-Resolved Study of Fluorescence Quenching of 9,10-Di(phenylethynyl)anthracene by Carbon Tetrabromide", C.E. Bunker, Y.-P. Sun, *J. Am. Chem. Soc.* **1995**, 117, 10865

"All-Carbon Polymers (Polyfullerenes) from Photochemical Reactions of Fullerene Clusters in Room-Temperature Solvent Mixtures", Y.-P. Sun, B. Ma, C.E. Bunker, B. Liu, *J. Am. Chem. Soc.* **1995**, 117, 12705

"Spectroscopic Investigations of Intermolecular and Intramolecular Eximers of Methylnaphthalenes and 1,3-Di(2-naphthayl)propane in Supercritical Carbon Dioxide", H.W. Rollins, R. Dabestani, Y.-P. Sun, *J. Phys. Chem.* **1995** (submitted)

"Ground State Charge Transfer Complexes of [84]Fullerene and N,N-Diethylaniline", C.E. Bunker, H.W. Rollins, Y.-P. Sun, *J. Chem Soc. Chem. Commun.* **1995**, (submitted)

Richard K. Marcus
Department of Chemistry
H.L. Hunter Chemistry Laboratory
Clemson University, Clemson, SC 29634-1905
Telephone: (864) 656-5011
FAX: (864) 656-6613
E-Mail: MARCUSR@clemson.edu

Education

B.S., Chemistry (with Honors) and Physics, Longwood College, Farmville, VA, 1982.
Ph.D., Analytical Chemistry (under Professor Willard W. Harrison), University of Virginia, Charlottesville, VA, 1986.

Research Interests

Development of instrumentation and/or methodologies for trace element analysis. Emphasis is placed on the use of glow discharge devices for atomic spectroscopic analysis and the study of their fundamental processes. Development of radio frequency powered glow discharge devices for the direct solids elemental analysis of non-conducting (insulating) sample types by optical and mass spectrometries. Application of collision induced dissociation (CID) strategies in glow discharge mass spectrometry. Use of ICR and ion trap mass spectrometers in atomic mass spectrometry. Use of glow discharge devices as metal ion sources for the study of gas phase inorganic chemistry. Liquid sample introduction into glow discharge devices via particle beam interfaces for atomic and molecular mass spectrometry. Investigations into the use of charge-injection devices as spatially selective detectors for dispersive mass spectrometry and ion imaging applications.

Honors

Clemson University Provost's Research Award
Invited participant, Emerging Scientists Symposium, 1994 Pittsburgh Conference
Clemson University Alumni Association Distinguished Researcher Award, 1994
Spectroscopy, Editorial Board "5 Brightest Stars in Analytical Spectroscopy", 1995

US Patents

Hollow Cathode Plasma Plume (with W. W. Harrison)

Radio Frequency Powered Glow Discharge Atomization/Excitation / Ionization Sources for Direct Solids Analysis, 6 granted (US and international), 1 pending

Presentations

Author / co-author of more than 60 refereed publications
Author / co-author of more than 190 conference presentations (30 invited)
Seventeen invited university/ national laboratory lectures
Editor- *Glow Discharge Spectroscopies*, Plenum, 1993

Professional

American Chemical Society (Analytical Division); member
American Society for Mass Spectrometry; member
Society for Applied Spectroscopy; Chairman, Piedmont Section
1995 FACSS Conference. Program Co-Chair
ICP Information Newsletter; Editorial Advisory Board
Spectrochimica Acta, Part B; Editorial Advisory Board
Journal of Analytical Atomic Spectrometry, Editorial Advisory Board
Applied Spectroscopy, Editorial Advisory Board
Jobin-Yvon, Division of Instruments SA; consultant

Mark C. Thies
Department of Chemical Engineering
Clemson University, Clemson, SC 29634
Telephone: (864) 656-5424
FAX: (864) 656-0784

Education

Ph.D., University of Delaware, 1985, Chemical Engineering
B.ChE., Georgia Tech, 1977, Chemical Engineering

Professional Experience

Clemson University, 1989-Present, Associate Professor of Chemical Engineering
Clemson University, 1985-1989, Assistant Professor of Chemical Engineering
Proctor & Gamble Company, Cincinnati, OH, 1977-1980, Process Development

Consulting Experience

Hoechst Celanese Corporation, Exxon Research and Engineering Company, United Nations Industrial Development Organization, Conoco Incorporated, Westvaco Corporation

Memberships

AIChE, ACS, American Carbon Society

Honors and Awards

Alexander von Humboldt Foundation Research Fellow (1994-1995)

Selected Publications

Brioncs, J. A.. Mullins, J. C., and Thies, M. C., Liquid-Liquid Equilibria for the Oleic Acid-β-Sitosterol-Water System at Elevated Temperatures, and Pressures, Ind. *Eng. Chem. Res.,* 33, (1994).

Stevenson, R. L-, LaBracio, D. S., Beaton, T. A., and Thies, M. C., Fluid Phase Equilibria and Critical Phenomena for the Dodecane-Water and Squalane-Water Systems, *Fluid Phase Equilibria,* **93**, (1994).

Bolanos, G., Liu, G.-Z., Hochgeschurtz, T., and Thies, M, C., Producing a Carbon Fiber precursor by Supercritical Fluid Extraction, *Fluid Phase Equilibria,* **82**, 303 (1993).

Hutchenson, K. W., Roebers, J. R., and Thies, M. C., Fractionation of Petroleum Pitch with Supercritical Toluene, J. *Supercritical Fluids,* **4**, 7 (1991).

Selected Research Grants (PI or Co-PI only)

"Engineering Feasibility Study," Conoco, Inc. (1994-1995), Principal Investigator (PI), $22,000.

"Supercritical Fluid Extraction for High Thermal Conductivity Carbon Fibers,' U.S. Army Research Office (1994-1997), PI, $297,000.

"Separation of Fischer-Tropsch Wax from Catalyst by Supercritical Fluid Extraction," U.S. Department of Energy (1994-1998), PI. $199,996.

"Polymer Fibrils and Microparticles by the Rapid Expansion of Supercritical Solutions." Industrial Sponsor (1993-1996), PI, $109,896.

Patents

"Solvent Extraction of Fatty Acid Stream with Liquid Water at Elevated Temperatures and Pressures," Thies, M. C., Mullins, J. C., and Briones, J. A., Inventors; March 17, 1992, No. 5,097,012.

Current and Past Graduate Students: 13

David S. Snipes
Department of Geological Sciences
Clemson University, Clemson, SC 29634
Telephone: (864) 656-5019
FAX: (864) 656-1041

Education

B.S., Wake Forest University, 1950
Ph.D., University of North Carolina, 1965

Professional Experience

1993-	Emeritus Professor of Geology
1979-93	Pofessor of Geology, Clemson University
1968-79	Assistant and Associate Professor, Clemson University
1963-68	Assistant and Associate Professor, Furman University

Other Related Experience

1968-93	Consutant, Hughes Well Drilling Co., State of South Carolina, HDR Engineering Co.; Berry, Dunbar, and Woods, Attorneys at Law; Carolina Well Drilling Co.;
1956-59	Petroleum Geologist, The California Company (now Chevron)
1950-53	First Lieutenant, Infantry, U.S. Army

Honors and Awards

Sigma Xi (1963)

Professional Societies

Geological Society of America
National Water Well Society
American Association of Petroleum Geologists
Carolina Geological Society

Publications: (1992-96)

Kroening, D., D. Snipes, S. Brame, R. Hodges, V. Price and T. Temples, "The Rehabilitation of Monitoring Wells Clogged by Calcite Precipitation and Drilling Mud", *Groundwater Monitoring and Review*, (in press), 1996.

Snipes, D. S., N.B Kidd,.R.D. Warner, R.A. Hodges, V. Price, Jr., and T. J. Temples, "An initial petrographic and geochemical study of a rhyolitic rock recovered from test well #I. Hilton Head, South Carolina", *South Carolina Geology*, **38**, p. 53-60,1995.

Warner, R. D., R. A. Hodges,. N. B. Kidd, D. S. Snipes, and J.C. Steiner., "Mafic mineral crystallization in South Carolina diabase", *South Carolina Geology*, **39**, p. 37-52,1995.

Kegley, W.P.,W.C. Fallaw, D. S. Snipes, S. M. Benson, and V. Price, Jr., "Textural factors affecting permeability at the MWD Well Field, Savannah River Site, Aiken, South Camrolina", *Southeastern Geology*, **34**, 139-161, 1994.

Fallaw, W. C., D. S. Snipes, and Price, V., Jr., "Wandering with William Bartram: the section at Silver Bluff, South Carolina", Earth Sciences History, **13**, 52-57 1994.

Current Research

Dr. Snipes is Principal Investigator on four research projects funded by US DOE and Westinghouse Savannah River Company (WSRC) through the South Carolina Universities Research and Education Foundation (SCUREF). Funding for the last five years totals more than $2,000,000, and current funding is $590,000. These projects involve eleven Clemson personnel including graduate students, research associates, and faculty.

John Steven Ramsdell
Marine Biomedical and Environmental Sciences
Medical University of South Carolina
Charleston, South Carolina 29412
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FAX: (803) 762-5535

Education

B.A. (Zoology) Drew University-1977
Ph.D. (Endocrinology) University of California, San Francisco-1982

Fields of Expertise

Toxicology of marine biotoxins including: their actions on signaling pathways that regulate the mammalian cell cycle, their action on intermediate response genes as an indicator of *in vivo* action and the development of novel detection methods based on their unique pharmacology.

Background / Work Experience

Research Fellow in Toxicology - Harvard School of Public Health. 1983- 1986.

Research Associate in Toxicology - Harvard School of Public Health. 1986-1987.

Acting Division Chief (Marine Biotoxins) - National Marine Fisheries Service, Charleston Laboratory 1992- present.

U.S. Delegation Member - IOC-FAO Intergovernmental Panel on Harmful Algal Blooms 1995-present.

Academic Experience and Affiliations

Assistant Professor- Department of Anatomy, Medical University of South Carolina. 1987-1992.

Associate Professor- Marine Biomedical and Environmental Sciences, Medical University of South Carolina. 1992-present.

Graduate Faculty - Molecular and Cellular Biology and Pathobiology Program, Medical University of South Carolina. 1987-present.

Graduate Coordinator- Marine Biomedical and Environmental Sciences, Medical University of South Carolina, 1992- present.

Adjunct Professor- Graduate Program in Marine Biology, University of Charleston, 1991-present.

NOAA Faculty Appointee- National Oceanic and Atmospheric Administration, 1992-1994.

Major and Recent Publications

Van Dolah, F.M., E.L. Finley, N.L. Zevotek, G.J. Doucette, P.D. Moeller and J.S. Ramsdell. 1995 Development of a sensitive, high throughput domoic acid receptor assay utilizing microplate scintillation technology. In: Lassus, P., Arzul, G., Erand, E., Gentien, P., and Marcaillou, C. (editors) Harmful Marine Algal Blooms, Lavoisier Science Publ. Paris 365-370.

Peng. Y.-G., T.B. Taylor R.E. Finch, P.D. Moeller and J.S. Ramsdell. 1995. Neuroexcitatory actions of ciguatoxin on brain regions associated with thermoregulation. *NeuroReport* **6**: 305-309.

Young, R.C., McLaren, M., and J.S. Ramsdell. 1995. Maitotoxin increases voltage independent chloride currents in GH_4C_1 pituitary cells. *Natural Toxins* **3**, 419-427.

Van Dolah, F.M. and J.S. Ramsdell. 1996. Maitotoxin activates type L dependent calcium channels, inhibits CDC2 kinase and progression through G2 of the cell cycle in GH_4C_1 cells. *Journal of Cellular Physiology* **166**, 49-56.

Robert J. Schalkoff
Department of Electrical and Computer Engineering
Clemson University, Clemson, SC 29634-0915
Telephone: (864) 656-5913
FAX: (864) 656-5910

Education

Ph.D., University of Virginia, 1979, Electrical Engineering
M.E., Rensselaer Polytechnic Institute, 1976, Power Engineering
B.S., University of Virginia, 1975, Electrical Engineering, with Highest Distinction

Professional Experience

Clemson University, 1989-present, Professor of Electrical and Computer Engineering
Worcester Polytechnic Institute, 1979-85, Associate Professor of Electrical Engineering
Exxon Production Research Company, 1976 -77, Engineer, Subsea Systems Section.

Relevant Publications

Schalkoff, R.J., "Digital Image Processing and Computer Vision", John Wiley and Sons, 1989.

Schalkoff, R.J., "Pattern Recognition: Statistical, Syntactic and Neural Approaches", (John Wiley and Sons, 1992).

Herwig, C.M., and Schalkoff, R.J., "Morphological Image Processing Using Artificial Neural Networks", *Digital Image Processing-.Techniques and Applications, Control and Dynamic Systems, Advances in Tbeory and Applications*, **67**, (C.T. Leondes, ed.), Academic Press, 1994, 319-379.

Mousavi, M., and Schalkoff, R.J., "ANN Implementation of Stereo Vision: Feature Extraction and Disparity Determination", *IEEE Transactions on System, Man and Cybernetics*, **24**, No. 08, August 1994.

Busboom, A. and Schalkoff, R.J, "Active Stereo Vision and Direct Surface Parameter Estimation: Curve-to-Curve Image Plane Mappings, accepted for publication in *Vision, Image and Signal Processing*, Oct. 1995.

Collaborators (Last 5 years)

M. Mousavi, K.A. Liburdy, S.M. Banks, C. Cox, S. Nugroho, R.D. Ferrell, U.M. Balasubramanian, C. Herwig, S. King, J. Millard. M. Kraess, A. Busboom, W. Sorge] , J.S. Byrd, J. Whitehouse.

Robert A. Fjeld
Environmental Systems Engineering
Clemson University, Clemson, SC 29634
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Education

Ph.D., Nuclear Engineering, The Pennsylvania State University, 1976
M.S., Minor in Air Pollution, The Pennsylvania State University, 1973, Nuclear Engineering
B.S., Nuclear Engineering, North Carolina State University, 1970

Professional Employment

1989-present, Professor; Environmental Systems Engineering, Clemson University
1980-89, Associate Professor; Environmental Systems Engineering, Clemson University
1976-80 Assistant Professor, Nuclear Engineering, Texas A&M University

Society Memberships / Professional Honors

Member, Health Physics Society

Member, American Association for the Advancement of Science

Member, American Nuclear Society

Member, ASME Mixed Waste Committee, Chair of Education and Information Subcommittee, Editor of Newsletter

National Academy of Sciences / National Research Council Committee on Decontamination and Decommissioning of Uranium Enrichment Facilities

National Academy of Sciences / National Research Council, Subcommittee on Decontamination and Decommissioning

Total Number of Refereed Publications - 31 (including 2 review artices)

Recent / Pertinent Publications

DeVol, T. A. and Fjeld, R. A. "Alpha/beta (gamma) Discrimination and Spillover Quantification with a BaF_2 Scintillator," *Nucl. Inst. Meth.*, **A253,** 28-32, 1994.

Fjeld, R. A., Guha, S., DeVol, T. A. and Leyba, J. D. "Ion Chromatography and On-Line Scintillation Counting for the Analysis of Non-Gamma Emitting Radionuclides in Reactor Coolant," J *Radioanal. and Nucl., Chem.*, **194,** 51-59, 1995.

Leyba, J. D., Vollmar, H. S., Fjeld, R. A., DeVol, T. A., Brown, D. D. and Cadieux, J. R. "Evaluation of a Direct Extraction/ Liquid Scintillation Counting Technique for the Measurement of Uranium in Water," *J. Radioanal. and Nucl. Chem.*, **194**, 337-344,1995.

Reboul, S. H. and Fjeld, R. A. "Effects of Surface Water Components on Actinide Determinations Conducted by Ion Chromatography," *Health Phys.*, **68**, 585-589, 1995.

DeVol, T. A., Brown, D. D., Leyba, J. D., and Fjeld, R. A. "A Comparison of Aqueous-Miscible Liquid Scintillation Cocktails with an Alpha/ Beta Discrimination Wallac 1415 Liquid Scintillation Counter," *Health Phys.* (in press).

DeVol, T. A. and Fjeld, R. A. "Development of an On-Line Scintillation Flow-Cell Detection System with Pulse Shape Discrimination for Quantification of Actinides at Environmental Levels," *IEEE Trans. Nucl. Sci.* (in press August 1995).

Ronald R. Williams
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H.L. Hunter Chemistry Laboratory
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Professional Experience

Acting Department Head, Clemson University, 12/93-8/94
Associate Professor of Chemistry, Ohio University, 9/87-8/88
Assistant Professor of Chemistry, Ohio University, 9/82-8/87

Research Interests

Fourier Transform Spectroscopy, Automated Instrumentation, Chemometrics

Education

B.S. in Chemistry (1977) University of South Carolina, Columbia, South Carolina

Ph.D. in Analytical Chemistry (1981), University of Georgia, Athens, Georgia
Thesis title: Fundamental Studies of Direct Current Plasmas
Thesis director: G.N. Coleman, University of Alberta, Edmonton, Alberta, Canada

Post-doctoral Fellowship (1982)
Topic: UV/ Visible Fourier Transform Spectroscopy
Under the direction of G. Horlick

Additional Experience

U.S. Environmental Protection Agency - development of GC/FTIR Spectroscopy for pollution analysis (1981), under the direction of-L. V. Azarraga

China Lake Naval Weapons Laboratory - Summer Research Fellow studying primary sources for atomic spectroscopy (1985), in collaboration with R. B. Green

Professional Activities:

Secretary of the Federation of Analytical Chemistry and Spectroscopy Societies
Treasurer Society for Applied Spectroscopy Piedmont Section

Michael L. Myrick
Department of Chemistry & Biochemistry
University of South Carolina, Columbia, SC 29208
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E-mail: myrick@psc.sc.edu

Professional Experience

1991 -present: Assistant Professor, Dept. of Chemistry and Biochemistry, University of South Carolina
1990-1991: Staff Scientist, Lawrence Livermore National Laboratory
1989-1990: Postdoctoral Research, Lawrence Livermore National Laboratory

Education

1985: B.S. in Chemistry, North Carolina State University (Raleigh, NC)
1985-1987: Graduate Study in Physical Chemistry, North Carolina State University (Raleigh, NC)
1988: Ph.D. in Physical Chemistry, New Mexico State University (Las Cruces, NM)

Honors/Awards

NC State Analytical Chemistry Award, 1985;
Fellow of the Microelectronics Center of North Carolina, 1985-1986;
NSF Fellow, 1986-1988;
Army Research Office Young Investigator, 1992-1995
Mortar Board Society Excellence in Teaching Award, 1994
South Carolina Honors College Outstanding Professor of Science, 1994.

Research Interests

Fiberoptic spectroscopy, applied chemistry, molecular excited state phenomena, nano-technology, scanning tunneling microscopy.

Recent Publications (total 60)

M. L. Myrick, N. V. Hud, S. M. Angel, and D. G. Garvis, "Tunneling spectroscopy on graphite:Implications for biological scanning tunneling microscopy," *Chem. Phys. Lett.* **180**, 156 (1991).

K. C. Yung, T. M. Vess, and M. L. Myrick, "Scanning tunneling microscopy of [Ru(1,10-phenanthroline)3]C12 on metals and GaAs: Electronic factors in imaging," in *Proc. Int.. Symp. on the Physics and Chemistry of Finite Systems: From Clusters to Crystals* (ed. by P. Jena, S. Ms. Khanna, and B. K. Rao), NATO ASI Series, Kluwer Academic Publishers, p. 1171 (1992).

J. D. Noll, J. B. Cooper, and M. L. Myrick, "A scanning tunneling microscopy study of HOPG defects," *J. Vac. Sci. Technol.* **A11**, 2006 (1993).

J. D. Noll, P. G. Van Patten, K. S. Booksh, M. A. Nicholson, and M. L. Myrick, "Flow injection system for the scanning tunneling microscope," *Rev. Sci. Instrum.* **66**, 4150 (1995).

P. G. Van Patten, J. D. Noll, M. L. Myrick, C.R. Li, and T. S. Sudarshan, "Spark-gap atomic emission microscopy," J. Phys. Chem. (in press, 1995).

TOTAL Research Assistants / Associates Supervised

Undergraduate 12
Masters: 0
Ph.D.: I0
Postdoctoral: 2

S. Michael Angel
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Education

Postdoctoral: Jan. 1985-1986, Department of Chemistry, Lawrence Livermore National Laboratory, Livermore, CA
Ph.D.: Dec. 1984, Analytical Chemistry, North Carolina State University, Raleigh, NC
B.S.: Dec. 1979, Chemistry, North Carolina State University, Raleigh, NC

Professional Experience

Aug. 1993-Present: Associate Professor of Chemistry, Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC 29208.

1989-Aug. 1993 Group leader, Advanced Measurement Sciences Group, Environmental Sciences Division, Lawrence Livermore National Laboratory, Livermore, CA.

1986-1989 Environmental Scientist, Environmental Sciences Division, Lawrence Livermore National Laboratory, Livermore, CA.

Research Interests

Applied Spectroscopy: Development of spectroscopic-based analytical methods, including remote spectroscopy and fiber-optic sensors, with emphasis on environmental applications and process chemistry.

Current Graduate Students

5 Ph.D., 3 Masters

Relevant Publications: (Total of more than 60 publications and book chapters)

S.M. Angel, M. Carrabba, and T.F. Cooney, "The Utilization of Diode Lasers for Raman Spectroscopy," *Spectrochim. Acta*. Part A, **51,** 1779-1799 (1995).

Thomas F. Cooney, H. Trey Skinner and S. M. Angel, "Evaluation of External-Cavity Diode Lasers for Raman Spectroscopy," *Appl. Spectrosc.*, **49,** 1846-1851 (1995).

R. E. Lyon, K. E. Chike, and S. M. Angel, "In Situ Cure Monitoring of Epoxy Resins Using Fiber-Optic Raman Spectroscopy," *J. Applied Polymer Science*, **53**, 1805-1812 (1994).

S.M. Angel, T. J. Kulp, M. L. Myrick, and K.C. Langry, "Development and Applications of Fiber Optic Sensors," in *Chemical Sensor Technology*, **3**, N. Yamazoe, Ed., Kodansha Ltd. and Elsevier Science Publishers, B. V. Amsterdam, 161-183 (1991).

S.M. Angel, B. L. Anderson, and K. Langry, "Simple Reversible Fiber-optic Chemical Sensors using Solvatochromic Dyes", in *Proceedings of SPIE OEIFibers 1991, Chemical, Biochemical, and Environmental Fiber Sensors III,* Boston, MA, **1587-15**, 86, September 3-6, 1991.

S. M. Angel, D. G. Garvis, S. K. Sharma, and A. Seki, "Field Applications of Fiber-Optic Sensors. Part I: Temperature Measurements in a Geothermal Well," Applied Spectroscopy, **43**, 430 (1989).

T. J. Kulp, I. Camins, S. M. Angel, C. Munkholm, and D.R. Walt, "Polymer Immobilized Enzyme Optrodes for the Detection of Penicillin", *Anal. Chem.*, **59,** 2849 (1987).

Christopher G. Kendall
Department of Geological Sciences
University of South Carolina, Columbia, SC 29208
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Education

Ph.D., 1966 (Sedimentology) Imperial College of Science, and Technology, London, U.K.
M.A., 1965 (Geology) Trinity College, Dublin
B.A., 1962 (1st Class Honors, Geology) Trinity College, Dublin

Professional employment

1988-present Professor in Department of Geology & Marine Science, USC (Tenured)
1986-present Dept. of Geology, USC. Professor (Tenured)
1983-present Dept. of Geology, USC. Professor (Untenurecl)
1982-1983 Gulf Research, Pittsburgh. Director Geol. Research
1981-1982 Gulf Research, Pittsburgh. Research Associate
1977-1981 Gulf Research, Pittsburgh. Senior Research Geologist
1977 Dept. Geology, USC. Research Assoc. Professor
1976-1977 Earth Science Resources, Associate Director. Inst.
1975-1976 Exxon Production Research, Research Specialist
1973-1974 Exxon Production Research Senior Research Geologist
1970-1973 Dept. Geol., Ohio State University, Assistant Professor
1970 Dept. Geol. Ohio State University Visiting Assistant Professor
1966-1968 Dept. Geology, University of Texas, Austin, Harkness Fellow
1962-1965 Dept. Geology, Imperial College, London, U.K., R. A.

Society memberships

Fellow of Geological Society of London
Member of Geological Society of America
Member Society of Economic Paleontologists and Mineralogists
Member of American Assoc. of Petroleum Geologists

Honors and awards

1985 Paper co-authored with Dr. J. K. Warren, "Disrupted carbonate hardgrounds in shallow carbonate-shelf sediments: origin and setting of tepees and their associated fabric" judged best of session at American Association of Petroleum Geologist Annual meeting.

1966 Harkness Fellow of Commonwealth Fund (One of thirty fellowships awarded annually in Britain to study in the USA).

Recent publications

Saidi A. Hassani, and Christopher G. St. C. Kendall, "Sedimentology and Alkaline Geochemistry of Rift Lake Manyara, Northern Tanzania, East Africa: An Analogue to Lacustrine Fill in Some Early Mesozoic Lakes of South East USA, *Southeastern Geology*, **34**, No. 3, 129-137 (1994)

Christopher G. St. C. Kendall, James L. Sadd, and Abdulrahman Alsharhan, "Holocene Marine Cement on Beachrocks of the Abu Dhabi Coastline (UAE)", *Analogs for Cement Fabrics in Ancient Limestones, Carbonates and Evaporites*, **9**, No. 2, 119-131 (1994)

Abdulrahman. S. Alsharhan and Christopher G. St. C. Kendall, "Depositional setting of the Upper Jurassic Hith Anhydrite of the Arabian Gulf: an analogue to Holocene evaporates of the United Arab Emirates and Lake MacLeod of Western Australia": *American Association of Petroleum Geologists Bulletin*, **78**, 1075-1096 (1994)

Robert Ehrlich
Department of Geological Sciences
University of South Carolina, Columbia, SC 29208
Telephone: (803) 777-6943
Fax: (803) 777-6610

Education

Ph.D., 1965, Louisiana State University
M.D., 1961, Louisiana State University
B.S., 1958, University of Minnesota

Professional Employment

1989-Present	Editor, *Mathematical Geology*
1974-Present	Professor, University of South Carolina
1969-1974	Associate Professor, Michigan State University
1965-1969	Assistant Professor, Michigan State University

Energy-Related Research Support from Non-Campus Sources

1988-1992 PADS, P.I.A. Research, $30,000
1990-1994 Canadian Hunter, Hydrocarbon Reservoirs, $63,000

Description of Current Energy-Related Research Projects

(1) Developing fundamental understanding of the porous microstructure with respect to multiple fluid phases
(2) Determining relationships between electrical conductivity and diffusivity in porous media
(3) Determining relationships between sample size, and physical properties of permeable media
(4) Prediction of permeability in sedimentary basins as a function of rock type and basin history

David E. Lincoln
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FAX: (803) 777-4002

Education

Ph.D., 1971, University of South Carolina
B.A., 1971, Kalamazoo College

Professional Employment

1991-Present	Professor, Biological Sciences, University of South Carolina
1986-1991	Associate Professor, Biological Sciences, University of South Carolina
1980-1986	Assistant Professor, Biological Sciences, University of South Carolina

Energy-Related MS Theses/Ph.D. Dissertations Supervised

S.A. Johnson, Ph.D./current, Variable plant response to herbivores under carbon dioxide and nutrient supplies

R.S. Williams, Ph.D./current, The impacts of elevated carbon dioxide and nutrient lamination on plant/insect interactions in pine and hardwood forest systems

C.S. Montjoy, MA/current, The effects of elevated carbon dioxide on the growth, reproduction and food consumption of *Melanoplus differentials and Melanoplus sanguinipes* feeding on *Andropogon ferardii*

K. Han, Ph.D./current, The evolution of carbon allocation to plant defense: a genetic analysis

Y. Liu, MA/current, Carbon supply effects on the chalcone synthase catalyzed production of flavonoids

Energy-Related Support from Non-Campus Sources

DOE, Herbivore responses to plants grown in enriched carbon dioxide atmospheres, $225,442 (1192-1995)
NSF, Chemically mediated interactions in a sedimentary assemblage, $240,000 (1992-1994)
NSF, Chemically mediated interactions in a sedimentary assemblage, $219,984 (1989-1992)

Description of Current Energy-Related Research Projects

Elevated atmospheric carbon dioxide significantly affects plan productivity and growth. Increased carbon fixation alters the carbon/nutrient content of leaves with subsequently influences many organisms, especially leaf-eating herbivores and decomposers. A major objective of my research is to understand how rising atmospheric C02 influences leaf-eating insects through declining leaf quality. Additionally, I am also interested in the production and biological influences of halogenated aromatic compounds, a major group of human pollutants, partly from energy production. Because they are also found in naturally occurring ecosystems, the goal of this program is to understand how these chemical function in unmanaged ecosystems.

Description of Energy-Related Industry/Laboratory Interaction Arrangements

Collaboration has been established with Dr. Richard Norby, Oak Ridge National Laboratory.

James R. Durig
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University of Missouri, Kansas City, MO 64110-2499
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FAX: (816) 235-5191

Education

Ph.D., 1962, Physical Chemistry, Massachusetts Institute of Technology
B.A., 1958, Chemistry, Washington & Jefferson College

Professional Employment

1993-Present	Dean, College of Arts & Sciences; Professor, Chemistry, UMKC
1973-1993	Dean, College of Science & Mathematics, University of South Carolina
1970-1973	Educational Foundation Professor of Chemistry, University of South Carolina
1969-1970	Professor of Chemistry, University of South Carolina
1965-1969	Associate Professor of Chemistry, University of South Carolina
1962-1965	Assistant Professor of Chemistry, University of South Carolina

Energy-Related Ph.D. Dissertations Supervised

Y.H. Kim, 1992, "Structural and Symmetry Determinations of Several Organoboranes Using Vibrational Spectroscopy and *Ab Initio* Calculations.

W.M. Zunic, 1992, "Pyrolysis Gas Chromatography/Fourier Transform Infrared Spectroscopy and Pyrolysis Gas Chromatography/Mass Spectrometry of Humic Acids, Indonesian Lignite and Bituminous Coals."

T.G. Costner, 1993, "Infrared and Raman Spectra, Conformational Stability, Barriers to Internal Rotation, Vibrational Assignment, and *Ab Initio* Calculations for Some Substituted Halopropenes".

Q. Tang, 1993, "Raman and Infrared Spectra Conformational Stability, Barriers to Internal Rotation, *Ab Initio* Calculations, and Vibrational Assignment of Some Halopropenes and Substituted Dimethyl Ether Molecules."

Energy-Related Publications

J.R. Durig, Q. Tang, and T.S. Little, "Raman and Infrared Spectra, Conformational Stability, Barriers to Internal Rotation, Vibrational Assignment, and *ab initio* Calculations of 3-Iodopropene". J. Raman Spectrosc., 23, 653 (1992)

J.R. Durig, T.S. Little, H.D. Bist, A. Rengan and J. Narayan, "Fourier Transform Raman Spectra of Diamond-Like Carbon Films", J. Raman Spectrosc., 23 625 (1992)

T.S. Little, X. Zhu, Aiying Wang, J.R. During, M. Dakkouri, T. Hermann, and O. Sala, "Spectra and Structure of Small Ring Compounds. LXI. Infrared and Raman Spectra, Vibrational Assignment, Conformational Stability and *ab initio* Calculations of Cyclopropylmethylsilane", Spectrochim. Acta, 49A, 2007 (1993)

M.S. Afifl, G.A Guigis, T.A Mohamed, W.A. Herrebout, and J.R. Durig, "Spectra and Structure of Silicon Containing Compounds. XVIII. Raman and Infrared Spectra, Conformational Stability, Vibrational Assignment. Barrier to Internal Rotation and *Ab Initio* Calculations of Ethyldichlorosilane, J. Raman Spectrosc., 25, 159 (1994)

H.D. Bist, S. Bhargava, T.S. Little, J.K. Gardner, Jr., J.R. Durig, S. Sahli, and M. Aslam, "Fourier Transform Raman Spectroscopy and Scanning Electron Microscopic Studies of Chemical Vapor Deposited Diamond-Like Carbon Films", J. Raman Spectrosc., 25, 67 (1994)

J.R. Durig, J.F. Davis and G.A. Guirgis, "Raman and Far Infrared Spectra, Structural Parameters and *Ab Initio* Calculations of Acetyl Chloride", J. Raman Spectrosc., 25, 189 (1994)

Arthur D. Cohen
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Education

Ph.D., 1968, Pennsylvania State University
B.S. 1964, University of Delaware

Professional Employment

1990-Present	Professor, Geological Sciences, University of South Carolina
1988-1990	Research Professor, Geological Sciences, University of South Carolina
1982-1988	Staff, Los Alamos National Laboratory
1975-1982	Professor, Geological Sciences, University of South Carolina
1974-1975	Professor/Staff, Geological Sciences, U. S. Geological Survey

Energy-Related Publications

Rollins, M.S., Cohen, A. D., and Durig, J. R., 1993, Effects of Fires on the Petrographic and Chemical Composition of eats in the Snuggedy Swamp of South Carolina, Int. Jour, Coal Geol., v.22, pp. 101-117.

Cohen, A. D., Davies, T. D., and Spackman, W., 1993 Sulfur Contents of Peats at the Confluence of Carbonate and Peat-forming Depositional Systems, Southeastern Florida: Proc. AAPG Eastern Sect. Mtg., p. 24.

Stack, E. M., Liu, J., Ives, J., Cohen, A. D., Durig, J. R., 1993, Characterized Peats as Sorption Media for Hazardous Waste Management V, v. II, Amer. Chem Soc., pp. 392-395.

Hoffman, G. K., Campbell, F. W., Beaumong, E. C., Kottlowski, F. E., Cohen, A. D., Kuellmer, F. J., Bellis, D., Cook, K. H., and Verploegh, J., 1993, Quality Assessment of the Strippable Coals in Northwestern New Medicao: Fruitland, Menefee, and Crevasse Canyon Formation Coals in the San Juan Basin, and Moreno Hill Formation Coals in the Salt Lake Field: New Mexico Bureau of Mines and Mineral Sources, Bull. 141, 84pp.

Energy-Related Support from Non-Campus Sources

1991-1992	Gasoline Contamination, Ground Water, EPA, $80,000
1991-1992	Coal Particle Grain Shape, EPRI, $33,000
1991	Patent Dev. Award, USC, $3,600
1992-1993	Upland Unit (w/ Colquhoun), DOE/SCUREF, $144,000
1992-1995	Coal Pet. Trop. Peat, NSF, $197,614

Description of Current Energy-Related Research Projects

My present energy-related projects include (1) development of an innovative method for refining and cleaning of crushed coal based on grain shape, (2) development of a method for clean-up of hazardous wastes (e.g., hydrocarbons from underground storage tanks and pipelines, metals and radionuclides from DOE sites), (3) dating the Upland Unit, a project focused on understanding the geologic formation on which all of the SRL reactors and burial sites sit, (4) basic research on the origin of coal macerals; (5) investigations of sulfur and mineral matter in coals and pears; and (6) studies of peats, coals and algae deposits as possible ancient-source rocks for petroleum.

Description of Energy-Related Industry/Laboratory Interaction Arrangements

I presently have links with (1) Westinghouse SRL (Rolf Adland, technical contact) to investigate the Upland Unit at the Savannah River Site; (2) Argonne National Laboratory, Chemistry Division (Gary Dyrkacz, coal origins); (3) Oak Ridge National Laboratory to support student's work under the traineeship program dealing with site-specific work at SRS.

Charles R. Lovell
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FAX: (803) 777-4002

Education

Ph.D., 1984, Microbial Ecology, Purdue University
B.S., 1979, Biological Sciences, Florida State University

Professional Employment

1993-Present Associate Professor, Biological and Marine Sciences, University of South Carolina
1987-1993 Assistant Professor, Biological and Marine Sciences, University of South Carolina 1984-1987 Postdoctoral Associate, University of Georgia

Energy-Related MS Theses/Ph.D. Dissertations Supervised

G. Lopez-de-Victoria, Ph.D./pending, "Chemoreception and chemotaxis of *Azospirillum* species to aromatic compounds"

Energy-Related Publications

"Motile behavior of *Azospirillum* species in response to aromatic compounds," submitted to Canadian Journal of Microbiology (with G. Lopez-de-Victoria, D.R. Fielder, and R.K Zimmer-Faust).

"DNA probes for the detection and identification of acetogenic bacteria," to appear in Acetogenesis, Chapman and Hall, New York.

"Purification and Properties of a homodimeric protocatechuate 4,5- dioxygenase *from Rhizobium leguminosarum,"* to appear in Archives of Microbiology (with Y.P. Chen).

"Purification of DNA from estuarine sediments," to appear in Journal of Microbiological Methods (with Y. Piceno).

"Utilization of aromatic compounds as carbon and energy sources during growth and N2-fixation by free-living nitrogen fixing bacteria," Archives of Microbiology, Vol. 59, 1993, pp. 2951-2955 (with G. Lopez-de-Victoria).

"Chemotactic behavior of *Azospirillum* species to aromatic compounds," Applied and Environmental Microbiology, Vol. 59, 1993, pp. 2951-2955 (with G. Lopez-de-Victoria).

Energy-Related Research Support from Non-Campus Sources

SCUREFIWSRC, "Development and improved methods for the use of functional group probes: Aromatic degraders", (1 9921994), $261,415

Description of Current Energy-Related Research Projects

Design, production, testing and field use of DNA probes specific to examine functional groups of bacteria in contaminated subsurface sediments. Responsiveness of soil bacteria to aromatic contaminants and the ability of these organisms to move to contaminated sites within soils is under investigation.- Current research efforts address probe sensitivity and amplification of specific nucleotide sequences from subsurface bacteria, as well as transport of bacteria within contaminated soils.

Robert L. Cannon
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University of South Carolina, Columbia, SC 29208
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Education

Ph.D., 1973, Computer Science, University of North Carolina at Chapel Hill
M.S., 1963, Mathematics, University of Wisconsin at Madison
B.S., 1961, Mathematics, University of North Carolina at Chapel Hill

Recent Professional Employment

1987-present	Professor and Chair of Department of Computer Science, University of South Carolina, Columbia, SC
1990-1991	Visiting Scientist, IBM Scientific Center, Palo Alto, CA
1984	Visiting Scientist, IBM Fellow Program, IBM Palo Alto Scientific Center, Palo Alto, CA
1983-1984	Visiting Professor, Computer Vision Laboratory, Center for Automation Research, University of Maryland, College Park, MD
1980-1983	Chair, Department of Computer Science, University of South Carolina, Columbia, SC
1973-1977	Assistant Professor of Computer Science, University of South Carolina, Columbia, SC
1968-1969	Assistant Professor of Mathematics, Wilmington College, Wilmington, OH
1967-1968	Instructor of Mathematics, Wilmington College, Wilmington, OH
1965-1966	Instructor of Mathematics, (Woodrow Wilson Intern), Philander Smith College, Little Rock, AR

Memberships

Association for Computing Machinery; IEEE Computer Society; Computing Sciences Accreditation Board

Recent Publications

Eberli, Gregor P., C. G. St.C., Kendall, P.D. Moore, G. L. Whittle, R.L. Cannon, "Testing a seismic interpretation of Great Bahama Bank with a computer simulation". American Association of Petroleum Geologists *Bulletin,* V. 78, No. 6, 1994, 981-1004.

Kendall, C. G. St.C., G. L. Whittle, R. Ehrlich, P. D. Moore, R. L. Cannon, and D. R. Hellmann, "Computer sedimentary simulation models sequence stratigraphy". *Oil and Gas Journal, 91,* 1993, 46-51.

Cheong, Dae-kyo, J. Strobel, G. Biswas, G. Lee, G.St.C. Kendall, R. L. Cannon, and J. C. Bezdek, PLAYMAKER: a knowledge-based expert system. *Geobyte,* V. 7, No. 7, 1993, 28-41.

Kendall, Christopher G.St.C., Gregorv Whittle, Phillip Moore, Robert Cannon, Douglas Hellmann, and Keith Spainhour, "The role of sedimentary simulations in stratigraphic analysis and their application to hydrocarbon exploration and production", in The Pohlman Report: Review of Geoscience Workstation Technology, V. 4, No. 6, November 1992, 44-57.

Kendall, Christopher G.St.C., Phillip Moore, Gregory Whittle, and Robert Cannon, "A challenge: Is it possible to determine eustasy and does it matter?", In, Dott, Robert H. Jr., ed., *Eustasy: The historical ups and downs of a major geological concept,* Geological Society of America, Memoir 180, 1992, 93-107.

Research Interests

Artificial Intelligence: expert systems for computer vision and geological exploration; Analysis of Algorithms: text collation and compression, Software Engineering: standardized development tools