

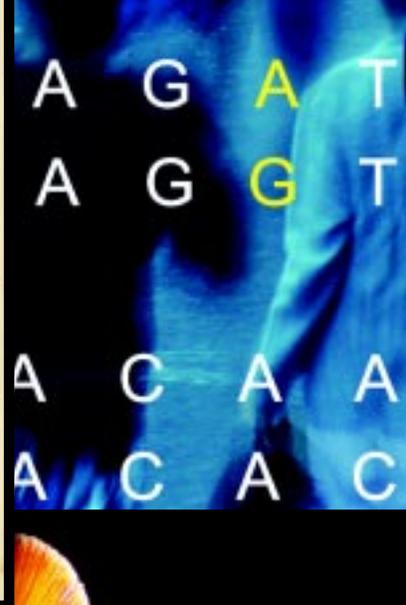
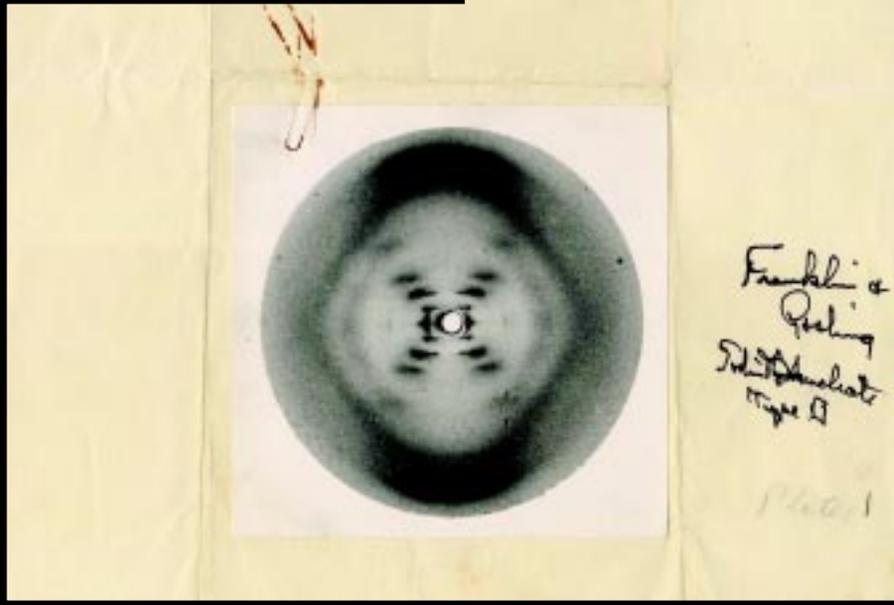
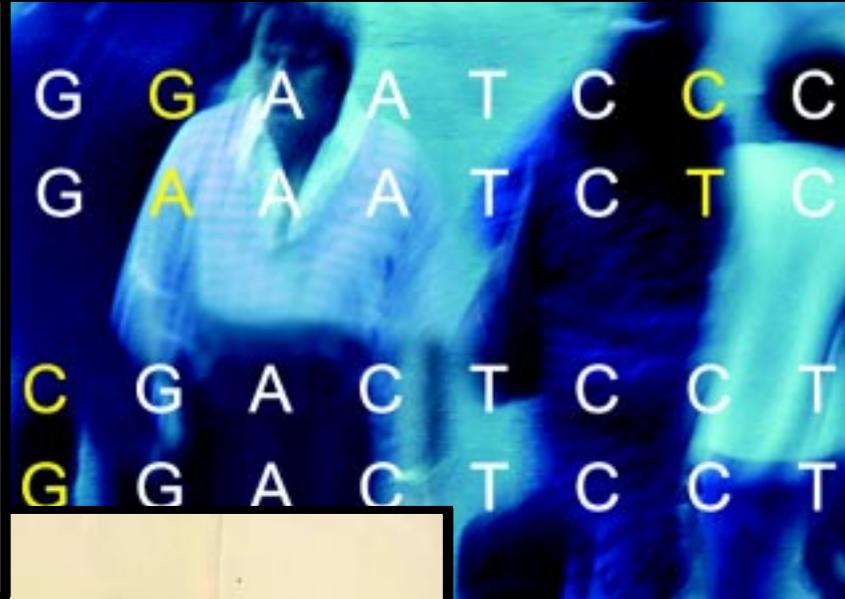
Journal of Undergraduate Research



U.S. Department of Energy



Office of Science



ABOUT THE COVER



Rosalind Franklin in the laboratory looking into a microscope. From *DNA: The Double Helix, Perspective and Prospective At Forty Years, 1953*. Original photograph by Henry Grant. Image used by permission of the Museum of London.

Sodium deoxyribose nucleate from calf thymus, Structure B, Photo 51, taken by Rosalind E. Franklin and R.G. Gosling. Linus Pauling's holographic annotations are to the right of the photo, May 2, 1952. Image used by permission of Special Collections, Oregon State University.



Grown from aqueous saline solution buffered with citrate at pH 7.3, this calf thymus DNA single crystal demonstrates birefringence and the beginning of a focal conic texture. The DNA concentration for this specimen is unknown but is presumed to be in the neighborhood of 400 milligrams per millimeter, and the magnification is approximately 200x. The digital image presented to the left was originally recorded on Fujichrome 64T transparency film using a Nikon Optiphot-Pol microscope with crossed polarized illumination.

Image courtesy Michael W. Davidson, National High Magnetic Field Laboratory, The Florida State University.

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A NOTE FROM THE EDITOR: SCIENTIFIC THOUGHT

Most professions seem to encourage certain approaches to the way their members think. This goes for brick layers as well as lawyers. One thing is for certain; scientists have a certain way of thinking. The challenge, even for scientists, is in identifying just what it is that sets us apart in our ways of thinking. The subject, on which numerous volumes have been written, is still quite unresolved. The first person I came across in my studies that seriously addressed this issue of scientific thinking or reasoning was a contemporary of Galileo, Francis Bacon. His aphorisms in the *Novum Organum* address many of the most difficult challenges in how we should go about thinking ... as scientists. One of my favorites can be summed up as: if science wants to advance, it must be willing to ignore what it assumes to be true. Being probably the first to fully attack the subject during a time when many “scientists” were as likely to practice astrology as astronomy, Bacon had his work cut out for him.

Surely, one of the trademarks of scientific thought is in the very word science derived from *scientia* (Latin ... knowledge) or *scire* (Latin ... to know). Notice the word does not mean “believe” (Latin ... *credo*). In the interest of setting our terms, which is a habitual concern of scientists, there is more than a fine difference between knowledge and belief. Knowledge is what we hold in our minds if it is true to the nature of the world, whereas belief need only be a resident of our minds with little natural fidelity. One of the marks of knowledge is how we cherish and preserve it, in stories, books and art. It is this drive to collect and preserve knowledge that in large part makes us human. In some respects then, science wishes to take humanity to another level through knowledge. There are different ways of knowing something. Science proposes to know nature a certain *way* and not necessarily at the exclusion of other *ways* such as religion or art.

Scientists choose to know the nature of the universe by observation and experimentation. When we feel we are far enough along, we form a theory which will typically have some value in its ability to predict nature. Some people¹ have been clever enough to point out that one test of whether a prediction is scientific is that it must be risky and specific. Attaching a prediction to something as dependable as the sun rising and setting is hardly risky, while vagueness can ascribe to predictions arising from knowledge for what belongs to chance. In the event that a theory is accurate and withstands years of testing in its predictions, it is often called a law. Some other clever people² point out that any scientific theory cannot actually be “proved” true and “falsifiability” is a signpost of scientific thought and a requisite for its theories. A particular theory, especially an appealing theory, is subject to constant verification through a variety of approaches. This could be called “proof by induction”, where enough cases have shown the theory holds true. During the constant process of verification the theory is vulnerable to disproof from a single well documented study. The point being that no amount of data and no number of studies can conclusively show the validity of a theory, while a single instance can conclusively reveal a theory as invalid. As scientists proceed through this process they look for causal (not casual) relationships and are keenly aware that correlation is not necessarily causation. Most theories cannot stand the onslaught and die quickly and/or quietly. Other theories that have held their ground for decades, as in Newton’s laws of motion, when found to be invalid, are invalid under circumstances that allow the basic theory to survive in a matured form.

There are central paradigms that scientists hold as immutable ... syllogistic reasoning for one. There are probably no “facts” of science that hold the same stature. Curiously, the greatest scientific thinkers have often been those willing to reject some of the most central of “facts”. Based on Kepler’s rejection of the circular motion of the planets,

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to advance, it
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true.**

Newton held Kepler in the highest regard. As a matter of human nature, people (scientists included) are not always kind to those who dare to think differently. This is understandable, even today. As a biologist, it is more than unsettling to watch some “facts” fall to the scientific method...all enzymes are no longer proteins, genes jump around in the genome, and a simple misfolded protein can be an infectious agent. These advances struck at some roundly accepted “facts” in biological science. Accepting these changes made for added complexity in the already overwhelmingly complex world of living systems. These thinkers did something somewhat distinctive to thinkers in and of science. They were willing to do as Bacon advised: ignore what science accepts to be true. Of interest here is that, in most every case I can think of where science advanced upon the rejection of an accepted “fact” the fact was, in fact, assumed from what seemed to be logical and obvious. Newton never said his laws applied to all frames of reference regardless of speed, and although we biologists became accustomed to the notion that all infectious agents are organisms and all enzymes were proteins, no experimental evidence excluded the other eventualities. We should have learned our lesson from viruses, which are NOT organisms.

One of the most confusing things to non-scientists is that scientists are seldom willing to completely trust their own facts, and seldom are scientists willing to accept something as beyond reproach. Probably the most defining characteristic of novel scientific thinking is the willingness to reject or ignore what seems obvious and factual and find a new way. Physics went through this reformation after quantum theory took hold and ushered in what is often called the “new physics”. No doubt other sciences will experience the same when thinkers of great thoughts find a new way to know nature.



Peter Faletra, Ph.D.
Editor-In-Chief

- 1) Karl Popper
- 2) Bertrand Russell, Karl Popper

THE VALUE OF MENTORING

“The notion of mentoring is ancient... In modern times the concept of mentoring has found application in virtually every forum of learning. In academics, mentor is often used synonymously with faculty advisor. A fundamental difference between mentoring and advising is more than advising; mentoring is a personal, as well as, professional relationship...In a broad sense, a mentor is someone who takes a special interest in helping another person develop into a successful professional.” (Advisory, Teacher, Role Model, Friend: On Being a Mentor to Students in Science and Engineering; National Academy Press; 1997)

Connecting students to the world of science and technology that exists beyond the academic classroom holds great potential for helping the students decide on and pursue a career pathway. Whether that path leads to a career in research, teaching, business, or a related scientific or technical field, the advanced scientific laboratories of the U.S. Department of Energy can enhance the knowledge and skills of undergraduates. This is accomplished by linking students to the research projects, facilities, instruments, and people found in these laboratories.

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If research and technology development are the essence of science and engineering, and a laboratory experience allows a student to see the process of science and engineering first-hand, then students in these disciplines can benefit from mentoring by laboratory scientists, engineers and technologists. Mentors are the essential guides and supporters of this learning experience, which differs from the science experience that most students have in a regular classroom setting.

For example, the DOE Community College Institute (CCI) of Science and Technology places community college students in internships in science, engineering and technology where they work directly with researchers. Luis Aceves, a Latino-American community college student from California participated in the CCI program at the Pacific Northwest National Laboratory (PNNL) in summer 2002. He is the first in his family to go on to college. He quit work in his father’s business in order to become a full-time student. Luis’s experience at PNNL

was his first research experience. His mentor, Michael Alexander, knew from experience that the initial stage of any student in his/her first research experience is “bewilderment.” The technologies and the protocols of actual scientific research were foreign to Luis, who actually stated, “What the heck did I get myself into?” Michael foresaw this reaction and explained to Luis that he was not concerned so much about what he knew but with what Luis could learn during the ten-week research experience. Michael designed a project for Luis that employed Luis’ immediate skills. Michael provided insights on how the technology worked in the research project and how a variety of disciplines are required for the research project to be successfully completed. Luis was provided technical manuals, virtual training courses, and classes that helped him learn the processes for conducting his summer research project. Michael introduced Luis to laboratory staff members who could offer

assistance and answer questions relating to his research project and who provided a network of professionals with whom Luis could interact. For his part, Luis had this to say about his relationship with Michael:

“My summer here was an awesome and very educational experience. I am thankful that he gave me the resources and trust to work on a part of his research I am most thankful that he chose me to be one of his fellows and for the opportunity to work with him. He made me feel every bit as important as the project itself. Michael was most interested in what I learned from the experience and in giving me ideas opportunities are in my future as a scientist. He made me feel like a professional colleague and gave me confidence in expressing my ideas on the experiments we conducted.”

Although mentoring is not the scientist’s or engineer’s primary responsibility, each staff member who agrees to enter into a mentoring relationship does so based on a common goal: to advance the educational and personal growth of the student. Students benefit from multiple mentors who represent diverse talents, ages, and personalities. While college and university faculty provide the core of the mentoring an undergraduate receives during her/his baccalaureate years, the opportunity to participate in a well-planned research project at a DOE National Laboratory can help the student better understand the practice of science and technology and add value to their education regardless of the career path they finally choose.

Thus, the laboratory staff member can become an important mentor to the student as well. In this role, the scientist or engineer can help the student 1) gain an appreciation for the many different careers in science and engineering, 2) realize that most careers are seldom a straight path to an imagined goal, but rather a series of “branching decision points” requiring an increasing degrees of flexibility and versatility, 3) develop important work habits and skills (e.g., communication, leadership, teamwork, and thinking skills), and 4) appreciate the special features, as well as the advantages and disadvantages, of a career in science and engineering. (NAP – 1997)

Young-Me Chung, a participant in DOE’s Science Undergraduate Laboratory Internship (SULI) Program had this to say about her mentor, Anna Gutowska:

“The human condition being what it is, the perfect mentor simply does not exist. However, Dr. Anna Gutowska comes very close. I greatly appreciated my mentor’s ability to balance lending me her support and expertise with challenging and entrusting me to accurately conduct lab work on my own and report the results with thoughtful analysis. Anna did not hold my hand, but if I tripped, she was ready to catch my arm before I fell flat on my face. She did not assign to me lab duties to perform blindly, but we discussed together the experimental approaches I would take and the principles behind them. She took my suggestions, questions, results, abstract drafts, and paper drafts seriously. Accordingly, I felt comfortable taking her feedback seriously.

Anna maintained a professional manner and a high level of expertise in her field of research, both in theory and in the lab. At the same time, Anna was a very warm and open person. Her

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enthusiasm was contagious (copolymers suddenly hold fascinations for me they never held prior to this summer!) and her communication skills were amazing. English is not her first language, yet she has explained to me numerous technical matters with effective idiomatic language, humor, and clarity, be it a dense paragraph in one of the background papers she gave to me on my first day at the lab or the manifold steps to a synthesis. Moreover, she was a careful listener, giving me her full attention, a fact I appreciate very much when having to explain not-so-good news such as troubleshooting stubborn equipment or quirky experimental results.”

In its educational toolkit on mentoring (Putting the Pieces Together – 2002), the Pacific Northwest National Laboratory describes mentoring as a shared relationship in which both the mentor and student benefit. For the student, the relationship is developmental; for the mentor the relationship creates opportunities to influence the growth and success of the student. For example:

- ◆ The student learns strategies on how to function and succeed in the workplace, while the mentor clarifies roles, responsibilities and expectations for the student.
- ◆ The student becomes aware of career and professional opportunities, while the mentor develops a sense of pride in seeing the student learn about, focus on, and accomplish goals.
- ◆ The student receives guidance in dealing with challenges and problems, while the mentor evaluates and acknowledges the student’s potential.
- ◆ The student gains a sounding board for exploring career, educational, and professional options, while the mentor provides key guidance, answers critical questions, and acts as a role model.
- ◆ The student gains a valuable friend and confidant, while the mentor engages in personal “coaching” that lets the student know that “he/she can do it.”

The National Academies’ handbook on mentoring (NAP-1997) highlights some of the outcomes of a quality mentor/student relationship. Many of these can be realized through an educational appointment at a DOE National Laboratory. For example, the student:

- ◆ Enhances her/his knowledge and skills through introduction to cutting-edge science and technology,
- ◆ Accumulates laboratory and field research skills through “work-based” training that may eventually influence the hiring decisions of prospective employers, including DOE and its laboratories,
- ◆ Masters laboratory techniques, learns to think critically, practices problem solving strategies, and experiences the importance of patience and perseverance in the unpredictable context of research,
- ◆ Takes a big step on the path to becoming a part of the “next generation of scientists and engineers.”

The mentor:

- ◆ Shares life experiences, wisdom, as well as technical expertise,
- ◆ Develops his/her own professional and interpersonal skills,
- ◆ Experiences the personal satisfaction found in teaching,
- ◆ Receives recognition in the academic and scientific community for their mentoring efforts, and
- ◆ Grows personally from exposure to a new ideas and perspectives of a diverse set of students who participate in these DOE undergraduate programs.

Perhaps nowhere in the portfolio of undergraduate programs sponsored by the Office of Workforce Development for Teachers and Scientists is the need for effective mentors greater than the Pre-Service Teacher (PST) Program. For the past three summers, PST has provided summer research internships, for undergraduate students who plan

on teaching. For many, if not all of these students, working in research is a new and often intimidating experience. A thoughtful and prepared mentor can make a difference. Sherene Carter, a student at Idaho State University, had this to say about the impact of her mentor, Deanna Auberry:

“Intimidated by the description of my lab research this summer, I was a little frightened to get in the lab. I had very little lab experience, and yet wanted to look like I knew what I was doing. Well, I didn’t. But when I met my mentor I knew that everything would be okay. Deanna was the hippest and coolest of mentors. She let me know that mistakes were not the end of the world; she expected them, but as time went on, I would get more comfortable in the lab.

As the summer went on, I realized that science is a slow process. A simple experiment that should take one or two days can end up taking 3 weeks! I witnessed that first hand. It’s was also important to be creative. Deanna taught me the art of improvising with the equipment that is available to you. With the lack of money, it is not always possible to order every little convenience. You have to make do.

I enjoyed and valued the lab experience I gained this summer. I have indeed become comfortable in the lab and more confident of my skills. I look forward to setting up labs for my future students and helping them to have more lab experience than I did when I was their age. This program has been a blessing in my life for more reasons than one. I hope to be able to encourage other Idaho State students to apply next year!”

These student vignettes describe the powerful impacts of a DOE research experience with an effective mentor. I encourage student and scientist alike to experience the mentor/student relationship by participating in a DOE undergraduate program. To be successful, mentors and students must make the effort to know, accept, and respect the goals and interests of one another. In the end, they can establish an environment in which the student’s accomplishments and the mentor’s satisfaction are only limited by the extent of their scientific talents and their commitment to one another.

Jeffrey Estes
Pacific Northwest National Laboratory

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ARGONNE NATIONAL LABORATORY



Argonne National Laboratory (ANL) is a Department of Energy, Office of Science facility on 1,700 acres located about 25 miles southwest of Chicago. ANL was the country's first National Laboratory and focuses on research areas including nuclear reactor development, energy and environmental technology, biomedical and environmental research, and basic sciences research. Some of ANL's significant accomplishments include: (1) the development of many of the nuclear power reactor types in use today; (2) development and construction of large superconducting magnets; (3) pioneering work in cancer diagnosis and therapy; and (4) development of lithium-metal sulfide batteries for vehicle propulsion and peak-load leveling for utilities. ANL is home to the Advanced Photon Source, a 1,104 meter circumference synchrotron-radiation light source producing high-brilliance x-ray beams used to carry out basic and applied research in the fields of biology, physics, chemistry, environmental, geophysical, and planetary sciences along with innovative x-ray instrumentation.

BROOKHAVEN NATIONAL LABORATORY



Brookhaven National Laboratory is operated by Brookhaven Science Associates for the Department of Energy, Office of Science. Located on a 5,300-acre site on eastern Long Island, New York, the laboratory operates large-scale facilities for studies in physics, chemistry, biology, medicine, applied science, and advanced technology.

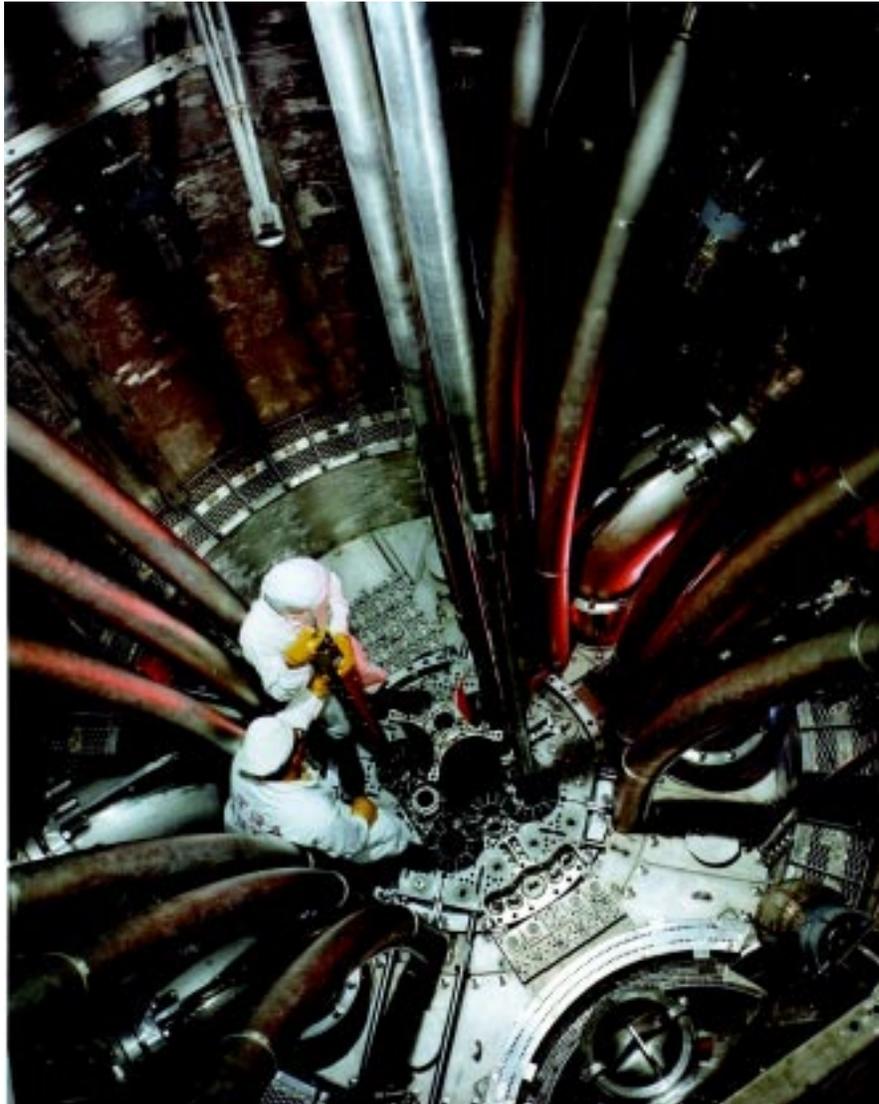
Brookhaven entered the 21st century with the world's newest and biggest particle accelerator for nuclear physics research, the Relativistic Heavy Ion Collider (RHIC). RHIC replicates conditions thought to have existed immediately following the Big Bang, to better understand subatomic particles and their interactions as well as how the universe evolved. Since Brookhaven was founded in 1947, five Nobel Prizes in physics have been won by scientists connected with the laboratory, including the 2002 Nobel Prize given to Raymond Davis Jr., for detecting solar neutrinos, ghostlike particles produced in the nuclear reactions that power the sun.

FERMI NATIONAL ACCELERATOR LABORATORY



Fermi National Accelerator Laboratory (Fermilab) is one of the world's foremost laboratories dedicated to high energy physics research. The laboratory is operated for the Department of Energy, Office of Science by a consortium of 89 leading research-oriented universities primarily in the United States, with members also in Canada, Italy and Japan. Fermilab is located on a 6,800 acre site about 45 miles west of Chicago. Fermilab is home to the Tevatron, the world's highest energy particle accelerator. Around its four-mile circumference 1,000 superconducting magnets are cooled by liquid helium to -268°C . Two major components of the Standard Model were discovered at Fermilab—the bottom quark and the top quark—and the first direct observation of the tau neutrino, the last fundamental particle to be observed, was at Fermilab.

IDAHO NATIONAL ENGINEERING AND ENVIRONMENTAL LABORATORY



The Idaho National Engineering and Environmental Laboratory (INEEL) is a multi-purpose national laboratory delivering specialized science and engineering solutions for the Department of Energy (DOE). The INEEL offers research opportunities in Generation IV Nuclear Energy Systems, National Security, Advanced Computing and Collaboration, Subsurface Science, Environmental Stewardship, Advanced Waste Management Solutions, Biotechnology, and Engineering.

The laboratory has been administered by DOE's Environmental Management Program and was recently reassigned to the Office of Nuclear Energy, Science and Technology. The INEEL, in partnership with Argonne National Laboratory-West, will become a major contributor to Generation IV nuclear energy systems and advanced proliferation-resistant fuel cycle technology. It is home to one of the largest concentrations of technical professionals in the northern Rocky Mountain region.

Located in southeastern Idaho, the INEEL covers 889 square miles of the Snake River Plain between Idaho Falls and Arco, Idaho. Offices and laboratories also are in the city of Idaho Falls (population 50,000), located about two hours from Grand Teton and Yellowstone national parks and other areas offering prime recreational opportunities.

LAWRENCE BERKELEY NATIONAL LABORATORY



Lawrence Berkeley National Laboratory's research and development includes new energy technologies and environmental solutions with a focus on energy efficiency, electric reliability, carbon management and global climate change, and fusion. Frontier research experiences exist in nanoscience, genomics and cancer research, advanced computing, and observing matter and energy at the most fundamental level in the universe. Ernest Orlando Lawrence founded the Berkeley Lab in 1931. Lawrence is most commonly known for his invention of the cyclotron, which led to a Golden Age of particle physics—the foundation of modern nuclear science—and revolutionary discoveries about the nature of the universe. Berkeley Lab's Advanced Light Source is its premier national user facility centrally located on the lab site overlooking the San Francisco Bay.

NATIONAL RENEWABLE ENERGY LABORATORY



The National Renewable Energy Laboratory (NREL) is the nation's leading National Laboratory for research and development in renewable energy and energy efficiency technologies. NREL's mission is to develop renewable energy and energy efficiency technologies and practices, advance related science and engineering, and transfer knowledge and innovations to address the nation's energy and environmental goals. NREL's research programs include basic energy research, photovoltaics, wind energy, building technologies, biomass power, biofuel, fuels utilization, solar industrial technologies, solar thermal electric, hydrogen, geothermal power, superconductivity, economic and policy analysis of renewable technologies, international development of renewable energy, and advanced vehicle technologies. *Research and Development*, *Discover*, *Scientific American* and *Popular Science* magazines have ranked many of NREL's research achievements among the nation's most significant technical innovations. NREL was recognized as one of the "Scientific American 50" for their contribution to science and technology. NREL was selected for their work in increasing the efficiency of photovoltaic solar cells. NREL's research into multi-junction solar cells has led the way to more efficient cells, offering the potential of cheaper electricity from the sun. Multi-junction solar cells use multiple layers of semiconductor material to absorb light and convert it into electricity more efficiently than single-junction cells. The cost of electricity from photovoltaic panels that convert sunlight directly into power has dropped from several dollars per kilowatt-hour, to 20-25 cents a kilowatt-hour today. NREL's 300-acre campus is nestled at the foot of South Table Mountain in Golden, Colorado.

OAK RIDGE NATIONAL LABORATORY



Originally known as Clinton Laboratories, Oak Ridge National Laboratory (ORNL) was established in 1943 to carry out a single, well-defined mission: the pilot-scale production and separation of plutonium for the World War II Manhattan Project. From this foundation, the laboratory has evolved into a unique resource for addressing important national and global energy and environmental issues. Today, ORNL pioneers the development of new energy sources, technologies, and materials and the advancement of knowledge in the biological, chemical, computational, engineering, environmental, physical, and social sciences. In addition, ORNL is responsible for the civil construction, project management, design integration, and ultimately the operation of the Spallation Neutron Source (SNS). Designed and constructed by a partnership of six Department of Energy National Laboratories (Argonne, Berkeley, Brookhaven, Jefferson, Los Alamos, and Oak Ridge), the SNS is a new, accelerator-based science facility that will provide neutron beams greater than ten times more intense than any other such source in the world. SNS will provide the opportunity for up to 2,000 researchers each year from universities, National Labs, and industry for basic and applied research and technology development in the fields of materials science, magnetic materials, polymers and complex fluids, chemistry, and biology.

PACIFIC NORTHWEST NATIONAL LABORATORY

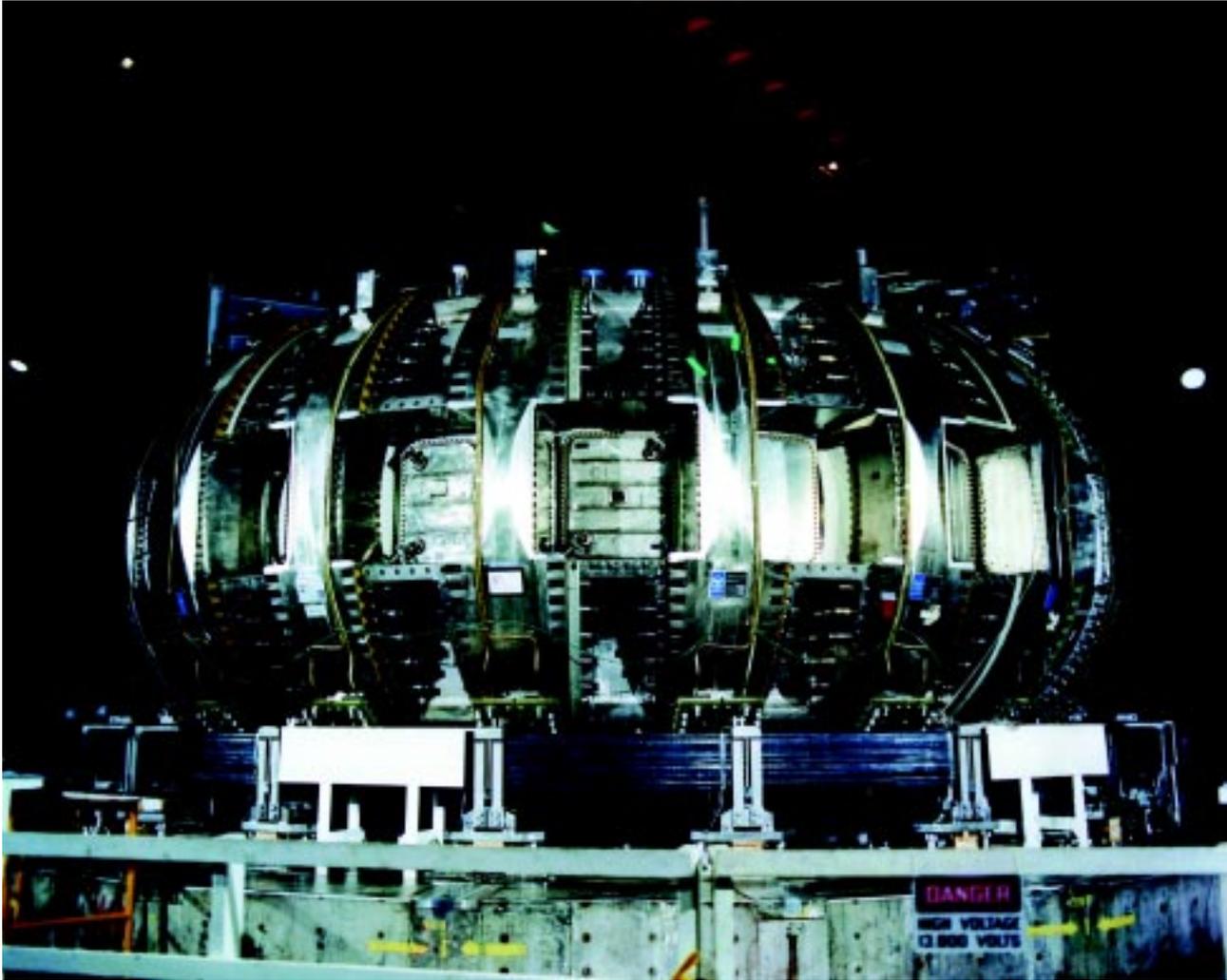


Pacific Northwest National Laboratory (PNNL) delivers breakthrough science and technology to meet key national needs. Pacific Northwest applies its capabilities to meet selected environmental, energy, health and national security objectives, strengthens the economy, and supports the education of future scientists and engineers.

Pacific Northwest is a world leader in environmental science research. The laboratory has built an international reputation in environmental sciences through fundamental studies in chemistry, biology, computer sciences, and a wide range of other fields. This expertise has been developed through an emphasis on understanding complex systems, from molecular to global scales. Research opportunities at the laboratory for students include appointments in atmospheric science and global change, computational sciences, experimental chemistry, marine sciences, molecular biology, environmental studies, remediation, environmental microbiology, wildlife and fisheries biology, materials research, process science and engineering, economics and political science.

PNNL is located at the confluence of the Columbia, Snake and Yakima rivers in southeastern Washington, the communities of Richland, Kennewick and Pasco.

PRINCETON PLASMA PHYSICS LABORATORY



The primary mission of the U.S. Department of Energy's Princeton Plasma Physics Laboratory (PPPL) is to develop the scientific understanding and the key innovations which will lead to an attractive fusion energy source. Associated missions include conducting world-class research along the broad frontier of plasma science and providing the highest quality of scientific education. Above is pictured the National Spherical Torus Experiment (NSTX), a proof-of-principle device that is testing the Spherical Torus (ST) plasma configuration. The ST concept could play an important role in the development of smaller and more economical fusion reactors. Including PPPL, the NSTX research team is comprised of 21 universities, National Laboratories, and research firms.

STANFORD LINEAR ACCELERATOR CENTER



The Stanford Linear Accelerator Center (SLAC) is one of the world's leading fundamental science research laboratories. SLAC designs, constructs and operates state-of-the-art particle accelerators and related experimental facilities used by physics studies probing the fundamental forces and structure of matter. The Stanford Synchrotron Radiation Laboratory (SSRL), a premier national user facility at SLAC, enables research requiring ultra high-intensity x-ray beams for molecular and atomic scale studies in physics, biology, chemistry, medicine, and environmental science. The BABAR collaboration investigating matter/anti-matter asymmetry is a current focus of high-energy physics, as is a vigorous R&D program focused on development of the Next Linear Collider, as part of a world-wide effort for this future facility. SLAC, operated by Stanford University for the Department of Energy, Office of Science, is 40 miles south of San Francisco, California.

THOMAS JEFFERSON NATIONAL ACCELERATOR FACILITY



Thomas Jefferson National Accelerator Facility (J-Lab) is a Department of Energy, Office of Science laboratory that uses advanced superconducting technology to accelerate a high energy, high current continuous electron beam. The electron beam begins orbiting in an underground racetrack containing a superconducting linear accelerator that drives electrons to higher energies. Magnets steer the beam from one section of the tunnel to another. After a few orbits, the electron beam is split for use in three simultaneous experiments. J-Lab is located in Newport News, Virginia.

Micha Kerr is currently enrolled as an undergraduate student at Roosevelt University in Chicago, where she is pursuing a B.S. in Environmental Science. Ms. Kerr accepted an appointment in the Environmental Sciences Division at Oak Ridge National Laboratory for the summer of 2002, through the Department of Energy's Community College Institute. Before her appointment, Ms. Kerr was studying at Jefferson Community College in Louisville, Kentucky. During her internship at ORNL, she studied and researched the bioremediation of brine-contaminated soils. Ms. Kerr pursues and promotes an environmentally sustainable culture and economy through research, writing, and active participation in our democracy.

Athur J. Stewart is an aquatic ecologist and ecotoxicologist, and received his doctoral degree from Michigan State University. At the time of this study, he was a senior scientist in the Environmental Sciences Division at the Oak Ridge National Laboratory in Oak Ridge, Tennessee. He retired from ORNL in 1993, but remains an adjunct research professor in the Department of Ecology and Evolutionary Biology at the University of Tennessee, Knoxville. In addition to publishing numerous scientific articles, book chapters and technical reports, many of his poems have been published in literary magazines and anthologies. His first book of poetry, *Rough Ascension and Other Poems of Science*, is scheduled for release late in 2003 through Celtic Cat Publishing.

TOLERANCE TEST OF *EISENIA FETIDA* FOR SODIUM CHLORIDE

MICHA KERR AND ARTHUR J. STEWART

ABSTRACT

Saltwater spills that make soil excessively saline often occur at petroleum exploration and production (E&P) sites and are ecologically damaging. Brine scars appear when produced water from an E&P site is spilled onto surrounding soil, causing loss of vegetation and subsequent soil erosion. Revegetating lands damaged by brine water can be difficult. The research reported here considers earthworms as a bioremedial treatment for increasing the salt mobility in this soil and encouraging plant growth and a healthy balance of soil nutrients. To determine the practical application of earthworms to remediate brine-contaminated soil, a 17-d test was conducted to establish salt tolerance levels for the common compost earthworm (*Eisenia fetida*) and relate those levels to soil salinity at brine-spill sites. Soil samples were amended with sodium chloride in concentrations ranging from 1 to 15 g/kg, which represent contamination levels at some spill sites. The survival rate of the earthworms was near 90% in all tested concentrations. Also, reproduction was noted in a number of the lower-concentration test replicates but absent above the 3-g/kg concentrations. Information gathered in this investigation can be used as reference in further studies of the tolerance of earthworms to salty soils, as results suggest that *E. fetida* is a good candidate to enhance remediation at brine-damaged sites.

INTRODUCTION

There are many damaging environmental problems related to the extraction of petroleum from the earth, not the least of which are brine spills. When oil deposits are tapped, petroleum isn't the only thing brought to the surface. For every barrel of crude oil produced, there are approximately 10 barrels of brine water produced (USGS 1997). Normally, this produced water is re-injected after it has been separated from the oil. However, when the water is spilled onto the surrounding land, a brine scar may appear after vegetation dies and soil is eroded, leaving a near-barren area. More than 2 billion gallons of brine water are re-injected each day into injection wells in the United States alone (USEPA 2002), and an indeterminate amount of this briny water is spilled annually. When the spills do occur, they can be very damaging to soil, plants, and soil biota; the damage can last for

decades. Data for the Tallgrass Prairie Preserve (northeast Oklahoma) may provide insight into the significance of brine spills, however. The Tallgrass Prairie Preserve (TPP) is 15,720 hectares (ha) in area, and contains some 337 oil wells. In association with oil extraction activities on the TPP, 126 brine spills have been reported. The total area of the brine spills is ~ 17 ha (Tom Ashwood, Environmental Sciences Division, ORNL, personal communication).

This brine water is more than just salt and water. Chemical composition of brine varies greatly from well to well and from oil-field to oil-field. Additionally, the salinity and constituents of co-produced water from a single site depends upon the depth from which the oil and water is being extracted. Of more than 57,000 samples of this water that the United States Geological Survey (USGS) has information on, the mean amount of total dissolved solids is 89.27 g/L, and the mean concentration of sodium ions is 28.36 g/L

(Breit 2002). Other ions such as bicarbonate, sulfate, potassium, magnesium, chloride, and calcium can be present at high concentrations as well (Breit 2002). In most cases, sodium chloride (NaCl) dominates ionic composition of briny co-produced water (Keiffer and Ungar 2001). For this reason, pure NaCl (rather than a mixture of salts) was used as the representative brine in the experiments reported here. The salinity levels of brine water vary greatly, from 1.0 g/L up to 400 g/L (USGS 1997). To put these levels into context, ocean water salinity is 35 g/L, and the NaCl limit for drinking water is 0.5 g/L (USGS 1997).

Part of the charge of oil producers and ecologists alike is to bring land scarred by brine water back into use or to its near-undisturbed state. Current techniques for achieving this goal focus on bioremediation, which generally refers to degradation of contaminants by living organisms. Bioremediation techniques are usually associated with microbes, but the practice can and does utilize other living things. The extent to which brine-contaminated soil can be remediated is yet to be fully seen, however, bioremediation has already been successfully addressing environmentally problematic incidents associated with the petroleum industry. In November, 2002, a proposal led by Dr. Kerry Sublette, University of Tulsa, was submitted to the Integrated Petroleum Environmental Consortium (IPEC) to address the question of how best to accelerate the restoration of oil- and brine-impacted sites using a combination of soil organic amendments, plants, and soil invertebrates. Studies and field trials have indicated that halophytes can remediate brine spill sites—at the very least, revegetate them (Keiffer and Ungar 2001, 2002).

This research examines the feasibility of using the earthworm, *Eisenia fetida*, as a potential bioremedial agent in the treatment of salty soils. Earthworms may facilitate increased salt mobility in soil and encourage plant growth and a healthy balance of soil nutrients. Earthworms also are good candidates because of their hardiness, as illustrated in this work.

Revegetating lands damaged by brine water can be difficult. Research on the tolerance of earthworms to salt is needed to assess the real potential of *E. fetida* to help restore brine-damaged soils. This study tests that potential.

MATERIALS AND METHODS

Endpoints of this bioassay were earthworm survival and reproduction. The species of earthworm chosen for this test was *Eisenia fetida*, or the common red worm (Edwards and Coulson 1992, Linz and Nakles 1997). The individuals were harvested from a culture kept on-site at Oak Ridge National Laboratory (ORNL) in Oak Ridge, Tennessee. The *Eisenia* cultures at ORNL were started in 1995 with juveniles obtained from East Tennessee State University (ETSU). The ETSU cultures, in turn, were started with individuals obtained from EPA (Region IV) in Atlanta, Georgia. A common, commercially available brand of topsoil (“Garden Basics”; South-

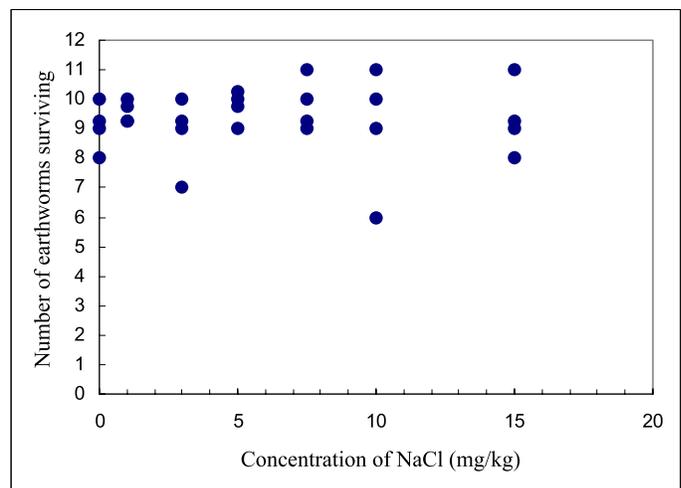


Figure 1. Survival of *Eisenia fetida* adults (17-d test) in soil containing various concentrations of NaCl. Eleven *E. fetida* were found in three replicates (one replicate each in the 7.5-, 10-, and 15-g/kg concentrations) at the end of the test; other replicates received 10 worms each at the start of the test. Data points are offsite slightly to allow the number surviving in each replicate to be determined.

ern Importers, Greensboro, North Carolina) was used for this test. Soil samples were weighed and dried at 60°C for 48 h, then reweighed to determine the water content of the soil.

Soil was treated with salt by application of solutions. The salt solutions were prepared using NaCl and deionized water. The tested concentrations of salt in soil (g/kg) were 0 (control), 1, 3, 5, 7.5, 10, and 15. Four replicate containers were used for each concentration. Each container received 50 mL of its assigned salt solution.

A 400-g quantity of soil (dry weight) was added to each replicate container that had been designed to allow aeration but prevent escape by the earthworms. The soil and test solutions were placed in these bags. Containers were then sealed and shaken before adding earthworms to facilitate the dispersion of the salt throughout the soil.

The earthworms were weighed in groups of 10 and added to the containers of test soil. All worms were incubated in beakers overnight to empty their guts before being weighed and placed into the test environments. After the earthworms were added, food (~2 g) was added to each container. The food consisted of Premium Rabbit Diet pellets (Pet Products; Hauppauge, New York), slurried into water (Gibbs et al. 1996).

Enough additional distilled water (25-75 mL) was added to each replicate to ensure moist but not saturated soil conditions. All replicates were allowed to incubate in a climate-controlled chamber at 25°C in darkness for 17 d. Replicates were periodically watered to maintain moisture levels friendly (moist to touch) to *E. fetida*.

At the end of 17 d, the replicates were disassembled and the worms counted and removed from the soil by hand. The recovered *E. fetida* again stayed overnight in beakers to

Salt Concentration (g/kg soil)	Y= Yes		N=No	
	Reproduction in Replicate Groups			
	A	B	C	D
0	Y	Y	Y	Y
1	Y	Y	Y	Y
3	Y	Y	N	N
5	N	N	N	N
7.5	N	N	N	N
10	N	N	N	N
15	N	N	N	N

Table 1. Evidence of *E. fetida* reproduction (Yes or No) in each replicate, for each concentration of salt tested. Evidence was “Yes” if juvenile worms or cocoons were observed, and “No” otherwise.

empty their guts before being weighed. The next day the earthworms were put into pre-weighed jars for drying. Next, the jars with the worms in them were weighed. They were then dried at 60°C for 6 d. After drying, the containers were weighed. (A weight subtraction adjustment of 0.09337 g was made to each empty vial weight in the calculation of earthworm dry weight to compensate for water lost from the vial’s cap. This number represents the mean difference between weights of wet and dry caps.)

The test soils were returned to their containers and again placed in the climate chamber. Three weeks later, the soil containers were emptied and hand-sorted to check for evidence of reproduction: the presence of juvenile *E. fetida*.

SUBTEST A

On day five of the test, a 0.5-g sample of soil was taken from each replicate, combined with the 0.5-g samples from the other replicates in its concentration class, and pH was measured. The 2-g soil samples from each test concentration were added to 50 mL of deionized water before the measurement was made.

SUBTEST B

On day seven of the test, a 50-g sample was taken from each replicate and added to 100 mL of deionized water. The sample was stirred, allowed to settle, and the conductivity was measured. Conductivity measurements were also made on NaCl solutions to establish a reference for comparison with the conductivities of the soil samples. Class concentrations of 0, 0.5, 1, 1.5, 2.5, 3, 3.75, 5, 7.5, 10, 15 g/L were tested using 100 mL samples of deionized water each.

SUBTEST C

In order to assess the influence of the earthworm food on the salt concentration in test soils, a conductivity measurement was made on control soils with and without food added. Neither sodium chloride nor earthworms were added to these test samples, and three replicates each were tested. Approximately 100 g of wet soil was used in each container; 1.6 g of food was added to three of the containers. All containers then received 50 mL of deionized water to disperse the food (where present). The samples were then covered and placed in a dark climate chamber at 25°C to ferment for 6 d to simulate feeding conditions of earthworm-containing soil replicates. On day six, 100 mL of deionized water was added to each replicate and conductivities were measured.

RESULTS

SURVIVAL

Earthworm survival (Fig. 1) was unaffected by the salt concentrations used in this experiment. The survival rate in replicates for the control soil ranged from 80%-100%. In replicates with a salt concentration of 1 g/kg soil, survival rates ranged from 90%-100%. Replicates with a salt concentration of 3 g/kg soil had a survival rate ranging from 70%-100%. At a salt concentration of 5 g/kg soil, survival rates ranged from 90%-100%. At 7.5 g of salt per kilogram of soil, survival rates ranged from 90%-100%. In replicates with a salt concentration of 10 g/kg soil, survival ranged from 60%-100%. In the replicates with the highest salt concentration (15 g/kg soil), survival ranged from 80%-100%.

Conductivity for soil extracts, per g of added NaCl, after correcting for background (105 μ S) (μ S)	NaCl concentration in soil (g/kg)	Conductivity ^a of water extract of NaCl-amended soil	NaCl concentration in pure water (g/L)	Conductivity of NaCl in pure water (μ S)
0	0	105 (90-120)	0	2
413	1	518 (405-684)	0.5	999
404.3	3	1318 (1084-1738)	1	1894
435.6	5	2283 (1960-2480)	1.5	2910
433.1	7.5	3353 (2630-3850)	2.5	3880
373.3	10	3838 (3300-4550)	3	5530
400.2	15	6108 (4120-7670)	3.75	6070
			5	9310
			7.5	13950
			10	16980

Table 2. Conductivity of various concentrations of NaCl in water, and of water extracts of NaCl-amended topsoil. To prepare water extracts of NaCl-amended soil, for each replicate, a 100 mL volume of deionized distilled water was added to a 50-g amount of soil.

REPRODUCTION

Cocoons were observed in many of the replicates upon breakdown. Successful reproduction (Table 1) occurred in all of the control and the lowest-concentration replicates and in half of the replicates containing NaCl at a concentration of 3 g/kg. No successful reproduction occurred in replicates with a salt/soil concentration above 3 g/kg. During the experiment, it was observed that the worms in replicates of higher salinities were much more sluggish throughout the experiment than the worms in lower concentrations of salt and the control. Some of the worms in a few higher-concentration replicates also exhibited escape behavior at the start of the test; they crawled out of the soil to the top seam of the container-bag and would have escaped if it had not been sealed.

pH

The pH measurements on the soil samples were found to be slightly acidic, ranging from 5.06-5.60. A marked drop in pH was noted between the 1 g/kg and 3 g/kg concentrations; it decreased from 5.5 to 5.15.

CONDUCTIVITY

A comparison of conductivities of soil replicates and salt solutions is presented in Table 2. The differences found in leachable salts from soil treated with and without food were very small. Untreated soil samples' conductivities ranged from 103-122 μ S and food-treated soils' conductivities ranged from 130.4-150.4 μ S.

DISCUSSION

The survival of *E. fetida* in this project speaks to their hardiness. Data obtained in this experiment indicate that

this species can tolerate soils nearly half as salty as seawater. This level of tolerance falls in line with the findings of Pearce and Pearce (1979, 1982), who noted that immersion in a solution half as salty as the sea was quickly fatal to several species of earthworms, while immersion in a solution one quarter as salty as seawater was tolerated. When viewed with results presented here, saltwater may be toxic to *E. fetida* at NaCl concentrations of 15-17 g/L.

There is, however, a difference between submerging earthworms in a saltwater solution for an acute test and confining them for longer periods to salty soils. Would the findings of Pearce and Pearce (1979) that *Lumbricus terrestris* and *Aporrectodea longa* were most tolerant to saltwater solutions accurately predict that those earthworm species would be most likely to thrive at brine spill sites? Findings here support that though they may not be the most saltwater-tolerant of earthworm species (Pearce and Pearce 1979), *E. fetida* have sufficient tolerance of salty soils to merit use at some produced-water spill sites.

Other studies have been conducted on the salt tolerance of invertebrates; the aquatic nematode *Caenorhabditis elegans* was shown to be quite tolerant in an acute test to salt solutions in concentrations of 15.46-20.5 g/L (Khanna et al. 1997). Hota and Rao (1985) found that the survival of three species of tropical earthworms (*Perionyz millardi*, *Octochaetona surensis*, *Drawida calebi*) was 50% (LC_{50}) in saline solutions of 9.5, 8.5, and 7 g NaCl per L, respectively. The study presented here suggests that North American *E. fetida* is more salt tolerant than the tested species of tropical earthworms.

Behavioral observations indicate that *E. fetida* may require a period of captive acclimation if they are to be used at higher-salinity field sites. As this 17-d tolerance test progressed, less escape behavior was observed. This leads the author to suggest that earthworms in captive or field conditions may acclimate. If allowed free range of mobility and travel, the earthworms may leave a test or field site

upon introduction. This does not rule them out as candidates as remediators because when contained, they seemed to adjust to the adverse conditions.

Evidence presented here also suggests that *E. fetida* cannot only tolerate lower-salinity soils, but also continue their natural life cycles. They can successfully reproduce in soils that may be representative of some soils at brine-damaged sites (Table 1).

Further investigation of the tolerance of *E. fetida* to salt and the effects of different soil types on this tolerance will be needed. A threshold concentration of NaCl for mortality and reproduction for this species will be useful if they are to be considered for field studies or as treatments for the bioremediation of site-specific brine-contaminated soils. A behavioral study could gauge the extent/intensity of their instinct to escape inhospitable soils. Investigation into the earthworms' ability to acclimate would provide information that could be directly applied to a field test or effort of bioremediating a brine spill site, indicating how long the creatures may need to be contained to an area or whether they would require the addition of uncontaminated soil to dilute sites of higher salinity.

Aside from the high concentrations of NaCl in produced water, the question remains, would *E. fetida* tolerate the concentrations of the myriad of other ions and compounds in the brine waters extracted at petroleum exploration and production sites. Information from the USGS's samples of produced water suggests that no two wells are chemical copies of each other. Are there elements in some of these waters that are acutely toxic to *E. fetida* in the soil environment? Further tolerance testing and field studies are called for to answer these questions.

CONCLUSIONS

With such a high tolerance to NaCl as seen in this investigation, *E. fetida* holds promise as a resource in the remediation of lands damaged by brine water at oil exploration and production sites. Differences in effects due to varying water and soil composition will require further investigation. Earthworms are an important segment of a healthy soil ecosystem; with their help, the application of bioremediation can keep us from taking the loss of surface earth with merely a grain of salt.

ACKNOWLEDGEMENTS

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James R. Wilson has been predicting the future for the US government for 26 years using probabilistic risk assessment. Part of his work involved predicting climate at the Yucca Mountain Nuclear Waste Repository one million years hence. Insights from this work led to five published papers on global climate prediction and the collaboration with Patrick Ray. Dr. Wilson is the manager of the Centre for Future Technologies, Inc .

LONG-TERM PREDICTIONS OF GLOBAL CLIMATE USING THE OCEAN CONVEYOR

PATRICK RAY AND JAMES R. WILSON

ABSTRACT

Many have attributed the Great Ocean Conveyor as a major driver of global climate change over millennia as well as a possible explanation for shorter (multidecadal) oscillations. The conveyor is thought to have a cycle time on the order of 1000 years, however recent research has suggested that it is much faster than previously believed (about 100 years). A faster conveyor leads to the possibility of the conveyor's role in even shorter oscillations such as the El Niño/Southern Oscillation (ENSO) and the North Atlantic Oscillation (NAO). The conveyor is primarily density driven. In this study the salty outflow of the Red Sea is used to predict its behavior ten years into the future. A successful model could lead to a long-term prediction (ten years) of El Niños, Atlantic hurricane season intensity, as well as global temperature and precipitation patterns.

INTRODUCTION

The Great Ocean Conveyor is a system of currents driven by thermohaline circulation that spreads heat, salt, and nutrients around the Earth (See Figure 1). Thermohaline circulation occurs largely in the North Atlantic, where, as water flows northward from the tropical Atlantic, evaporation is greater than precipitation, making the water saltier over time. In the North Atlantic the water cools as it gives off heat and the cooler, saltier water becomes more dense and sinks. The deep water then flows southward, eventually joining the Antarctic Circumpolar Current and spreading the water throughout the oceans (Musgrave, 2000). The resulting current system dwarfs the flow and size of any river system on Earth. The conveyor is a major driver of global climate. For example, Europe experiences a much warmer climate than regions at the same latitude because of the heat it receives from the warm northerly flowing conveyor in the North Atlantic (Gray, 1998).

Traditionally, the conveyor cycle time is thought to be on the order of a thousand years, precluding it from affecting short-term climatic oscillations such as the El Niño/Southern Oscillation (ENSO) and the North Atlantic Oscillation (NAO). ENSO and NAO are believed to be affected by the conveyor on multidecadal scales (Gray, 1998). Research in-

dicating that shorter oscillations (2 to 8 years) are linked to the conveyor has not been located. New research suggests that the cycle time of the conveyor is much faster, about 100 years (Wilson, 2001), allowing the conveyor to be a more active player in short-term oscillations. The conveyor is sensitive to changes in salinity, and Wilson suggests that the ultra-saline Red Sea may play a major role in the behavior of the conveyor (Wilson, 2001). Recently Red Sea water has been found in eddies rounding the tip of Africa (Philippens, 2001). The area lies along the path of the conveyor and shows that Red Sea water is indeed picked up by the conveyor.

We suggest that the flow of the conveyor affects short-term climatic oscillations such as those found in ENSO, NAO, Atlantic hurricane activity, as well as typical temperature and precipitation trends around the globe. We also suggest that an oscillating volume of salt entering the conveyor from the Red Sea causes salinity changes which in turn cause the short-term oscillations.

The outflow of the Red Sea is not constant. More salt enters the Gulf of Aden and eventually the Indian Ocean when winds blow from the Gulf of Aden into the Red Sea. When this happens, a two way flow is set up through the Bab el Mandab Strait sending Red Sea water into the Gulf of Aden where it is picked up by the conveyor. The winds in

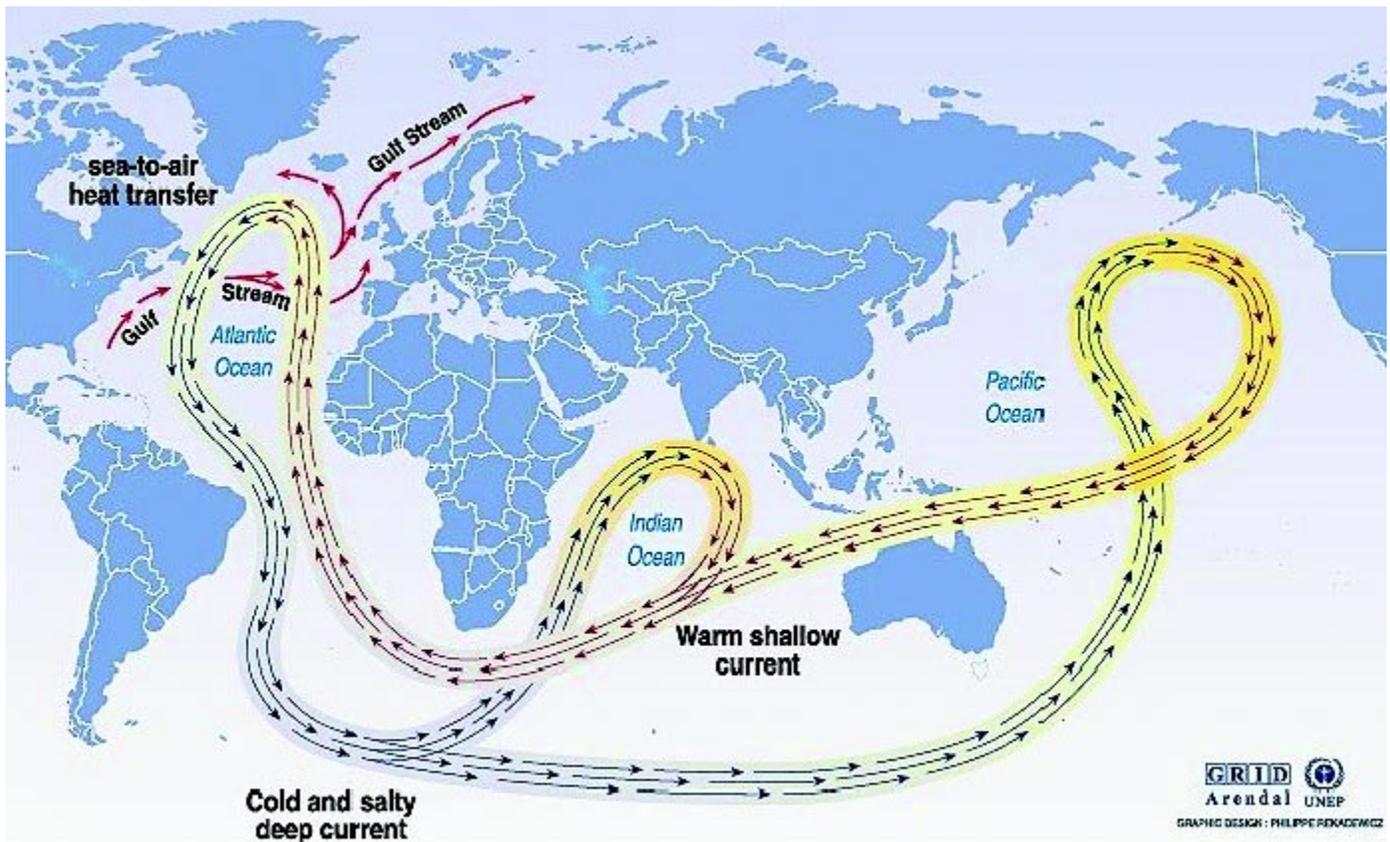


Figure 1: Great Ocean Conveyor Belt

the area are monsoonal and during tor that governs how much salt enters the conveyor from the Red Sea. (see Figure 2)

Salt exiting the Red Sea would most likely not have an immediate effect on the conveyor, because in areas where the conveyor runs “smoothly” a change in salinity has negligible effects. However, at certain points along its journey, it is likely to encounter places where a small salinity change could greatly increase or decrease the flow of the conveyor. We consider the conveyor to act as a train, meaning an increase or decrease in speed in one area will cause a similar result, or at least affect the flow in other areas. The dynamics of how different parts of the conveyor affect each other are unknown.

The goal of this work was to create a simple model intended to predict the behavior of the conveyor over time. As salt “bumps” come out of the Red Sea, they can be tracked through weather stations around the globe, and at certain points oceanic and atmospheric reactions (such as El Niño) can be consistently observed. Though our assumed cycle time of the conveyor is much shorter than the accepted cycle time, it is still fairly long and salt bumps are present for many decades. Therefore, we believe it is possible to use the salt bumps to make long-term predictions of conveyor behavior.

A successful model would help guide other researchers who may be able to improve upon the model. The accurate

prediction of events such as El Niños, droughts, floods, heat waves, and cold spells ten years in advance has enormous economic implications. Current computer models run by supercomputers are only reliable for short-term predictions (a few months). A ten year prediction run by a simple spreadsheet would certainly be an achievement.

METHODS

A monthly time series of wind speed and direction in Northeastern Africa was sought. Unfortunately the area does not have many weather stations and those that exist are often poorly maintained. However, there was a station that operated between 1902 and 1991 with a monthly time series of precipitation. Djibouti is an African city in the country of the same name. It is located on the western tip of the Gulf of Aden, very near the Bab el Mandab Strait and therefore, well placed to use as a resource for local weather patterns. The area is a desert with little rainfall, however the rain that does fall follows a well-defined pattern (Climate, 2002). Most of the rain falls between October and April when the winter monsoonal winds carry in moisture from the ocean; these same winds drive the salt out of the Red Sea into the ocean. Djibouti rainfall is therefore used as an indicator of salt volume exiting the Red Sea (see figure 2).

The Southern Oscillation Index (SOI) is defined as a

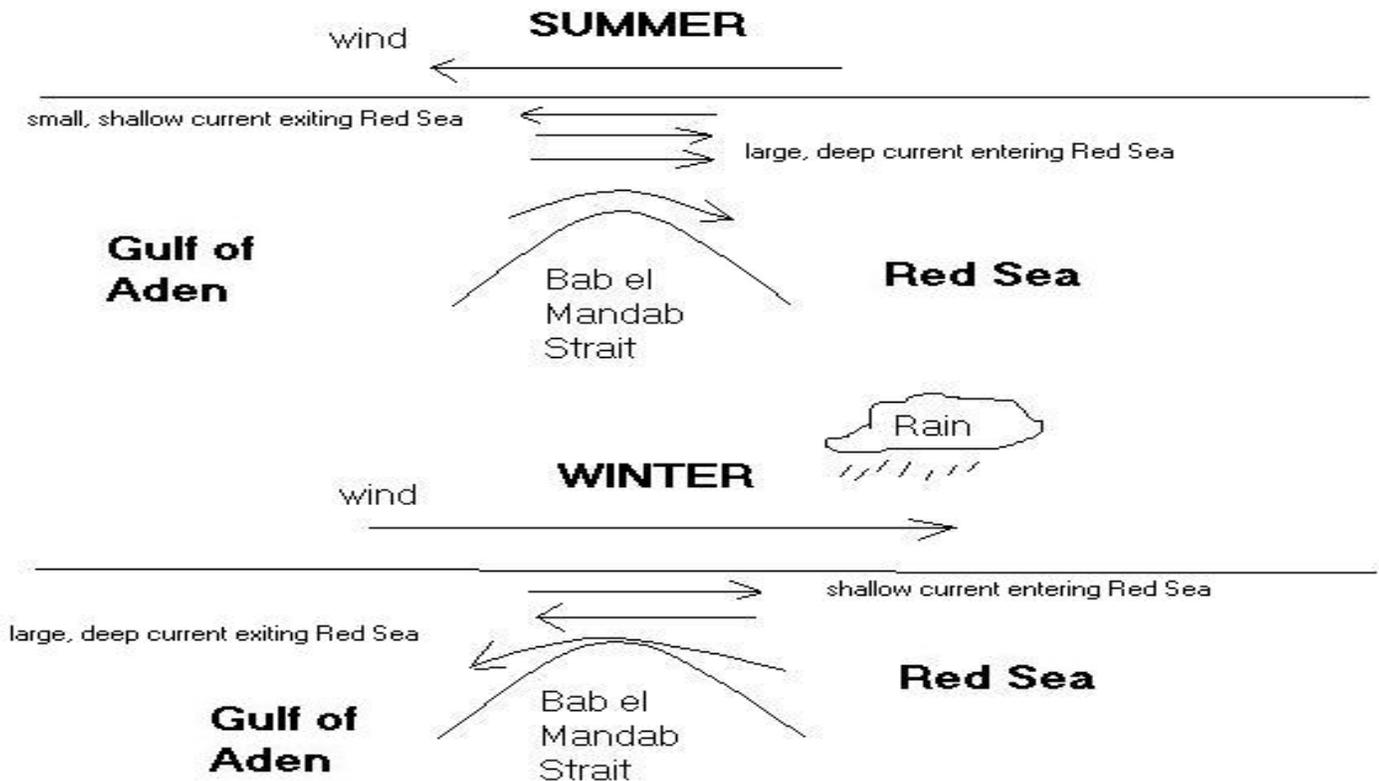


Figure 2: Seasonal Red Sea Outflow Cycle

normalized atmospheric pressure difference between weather stations on the island of Tahiti and at Darwin, Australia (SOI, 2001). The SOI is commonly used as a measure of ENSO (Daley, 2002). If ENSO is caused by changes in the conveyor, and the SOI is a good measure of ENSO, then the SOI also is a good measure of conveyor behavior. Since the conveyor works as a train its geographic location is of little importance. The SOI monthly time series has the advantage of having data from 1866 until the present with no missing values.

The time consuming part of the research involved finding where the salt "bumps" alter the flow of the conveyor. By looking at Sea Surface Temperature (SST) anomalies, we noticed that before the onset of an El Niño a cold SST anomaly appeared on the Atlantic side of southern Africa and a warm SST anomaly occurred southeast of the Cape of Good Hope (See Figure 3). In this area the warm Agulhas Current carries warm water around the tip of Africa, but the current comes very close to the much larger Antarctic Circumpolar Current. The cold water anomaly off of the west coast of Africa and the warm water anomaly to the southeast of the Cape of Good Hope suggest that warm water is no longer rounding the tip of Africa (meaning the conveyor has slowed or stopped). Air temperature data from Luanda confirmed a correlation with the SOI (see Figure 4). A graph

of Luanda temperatures resembles the graph of SOI over time, however Luanda temperatures precede the SOI. Though they do not precede the SOI by much (approximately 1 year), this fact seems to indicate that the initial reaction to a change in the conveyor happens far west of the Pacific. As time goes on, warm water piles up in the Indian Ocean as if a dam were thrown into the conveyor. This causes a buildup of warm water that extends eastward with time. At some point, the warm water piling up in the Indian Ocean seems to trigger the atmospheric domino effect, resulting in an El Niño.

The observation still does not tell us where the conveyor slows or stops, it merely tells us what happens when it does. The lags, the time between a salt bump exiting the Red Sea and its having an observed effect, were found simply by matching data. We attempted to match the SOI with Djibouti rainfall (indicator of salt) from past years. The lag producing the best fit then became our crude model. We then took the residual of the model and compared it to Djibouti rainfall at different lags. The lag that produced the best match to the residual was then mathematically scaled for best fit and added to the first model to create an improved model. The residual from the new model was then found and matched with yet another different lag, creating a model that incorporated three lags.

RESULTS

The lags were found to be 10, 35, and 13.5 years respectively. The 35 year lag is thought to be the downwelling point in the North Atlantic. This would lead to an approximate average speed of 0.07 mph for the conveyor. A one thousand year cycle time for the conveyor would lead to a half cycle of slightly less than 500 years for the short loop through the Indian ocean, and an approximate average speed of .001 mph. Some currents such as the Agulhas Current, which is part of the conveyor, can reach speeds of more than 4 mph (Agulhas, 2002), so even the faster conveyor is very slow compared to some of the currents through which it propagates. The 10-year lag is thought to correspond to area around the Cape of Good Hope where the Agulhas, the Benguelas, and the Antarctic Circumpolar Currents all meet. The reasons for the 13.5 year lag are unknown. A change in salinity has some effect on the flow of the conveyor at each time location corresponding to a lag. The initial fit was calculated using SOI data from 1940-1970 compared to Djibouti

rainfall from years prior to that. The danger of this type of modeling is over-manipulation of the data (i.e. matching data together after the fact proves nothing). Our initial hope was to show a salt oscillator could produce variations of the correct frequency as those observed for ENSO. After manually fitting the short-term oscillations for 1940-1970, the model was expanded without alteration for the rest of the time period. Not surprisingly, the short-term oscillations did not generally fit for all time periods (See figure 5). However, according to trendlines created by Microsoft Excel (labeled "poly" on figure 5), the model's long-term oscillations matched those of the SOI for all time periods despite the fact that no effort had been made to fit long-term oscillations.

Encouraged by the model's relative success at predicting long-term oscillations, we sought out to find out why the short-term oscillations did not fit. The short-term oscillations seemed only to be off during the time period 1976-1991. On further investigation, it was found that the structure

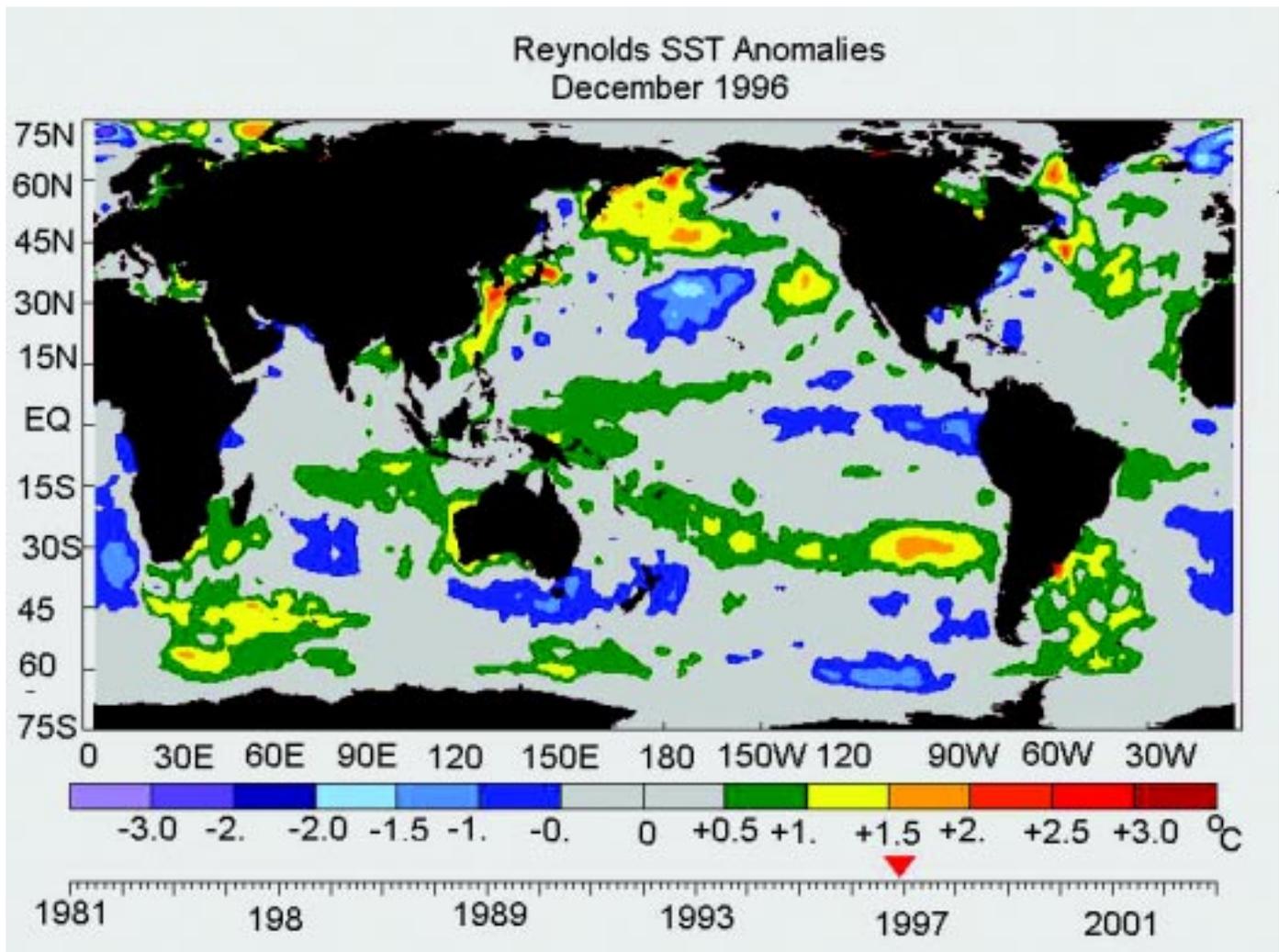


Figure 3: Water Temperature Anomaly

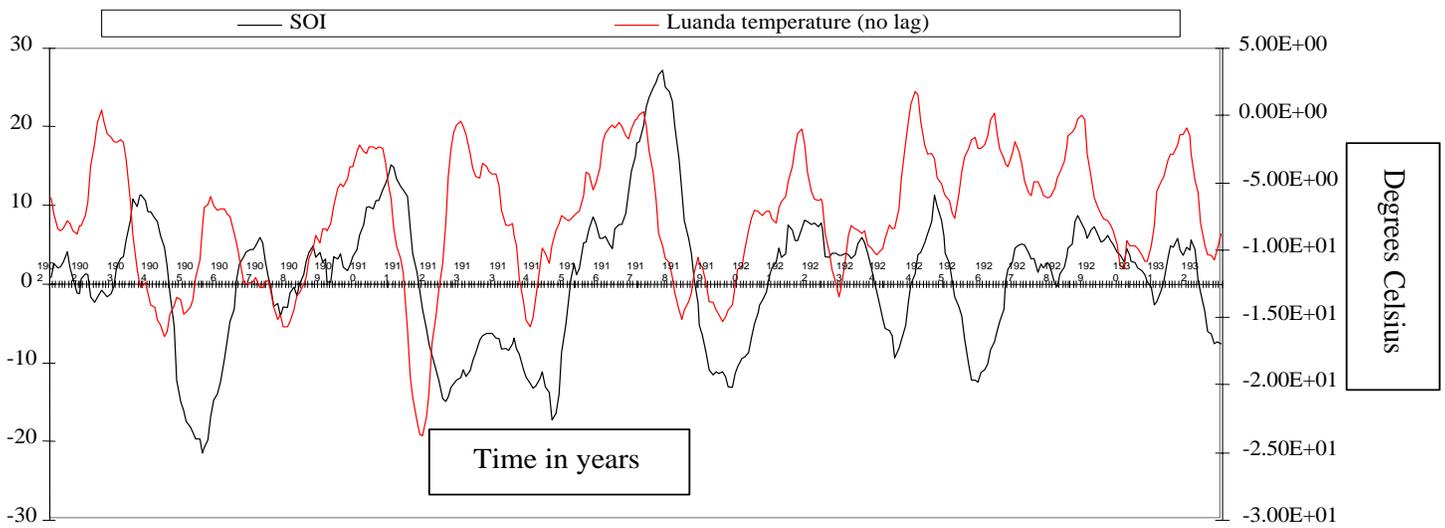


Figure 4: Luanda Temperature v. SOI. Temperature anomalies in Luanda, Africa plotted against the SOI. Note that Luanda temperatures tend to lead the SOI.

was still correct, but the SOI had suddenly shifted to become out of phase with the model by 2 years (i.e. proper lags would now be 8, 33, and 11.5 years, respectively) (see figure 6). This would indicate an increase in the speed of the conveyor during these years. This time period matched the “Great Pacific Climate Shift,” a period in which global temperatures very suddenly rose (Beliunas, 2002) (see figure 7). The reasons for this shift are unknown and the model failed to predict it, however the model simply measures the input from the Red Sea. Many other factors may affect the conveyor.

When the model was manually adjusted for the “Great Pacific Climate Shift,” the model accurately predicts long-term and, to a lesser extent, short-term oscillations in the SOI (see figure 8). The model enables predictions to be made 10 years into the future. Unfortunately the time series in Djibouti ended in 1991, allowing the model to predict only until 2001. A monthly time series of precipitation in Ethiopia has been used to extend the model, however it is too early to tell whether it will be as successful as the Djibouti data.

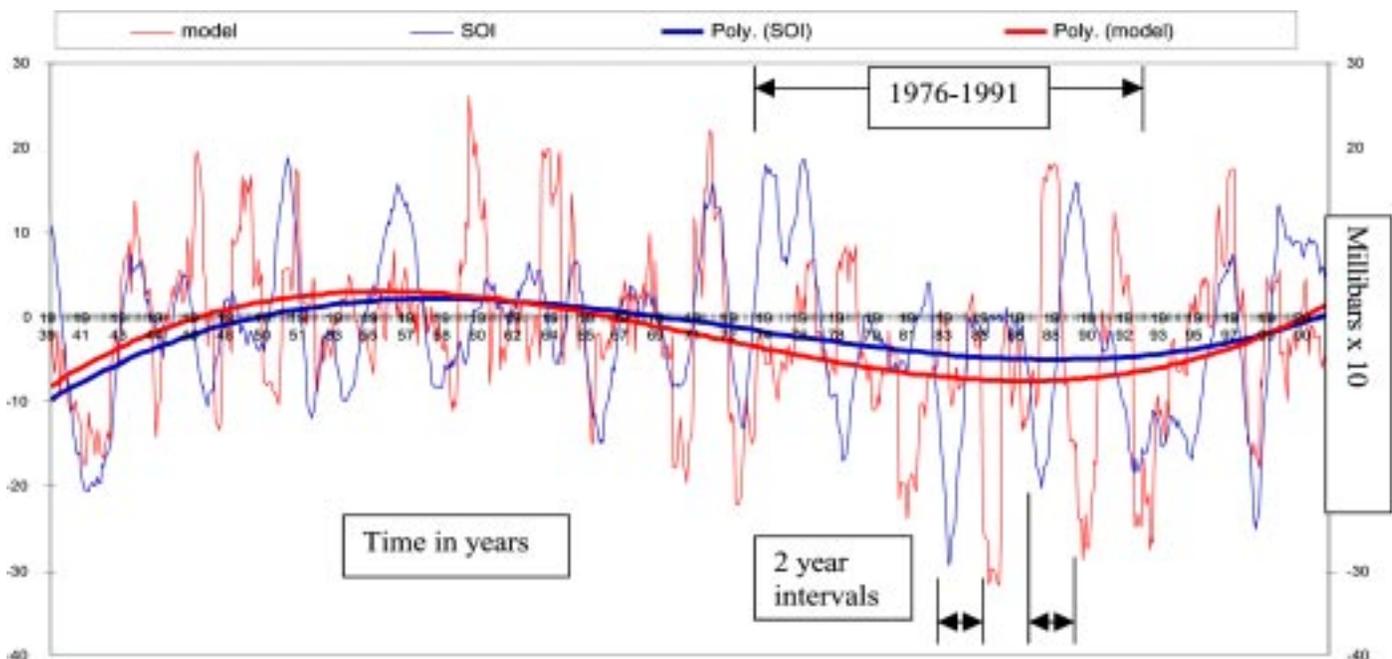


Figure 5: SOI Model v. SOI Actual. Model outputs before any manual adjustments are made. Trendlines show long-term oscillations. Note that the short-term oscillations also fit for all times except for between 1976 - 1991. During this time period the Great Pacific Climate Shift occurred, and the graph becomes out of phase by 2 years.

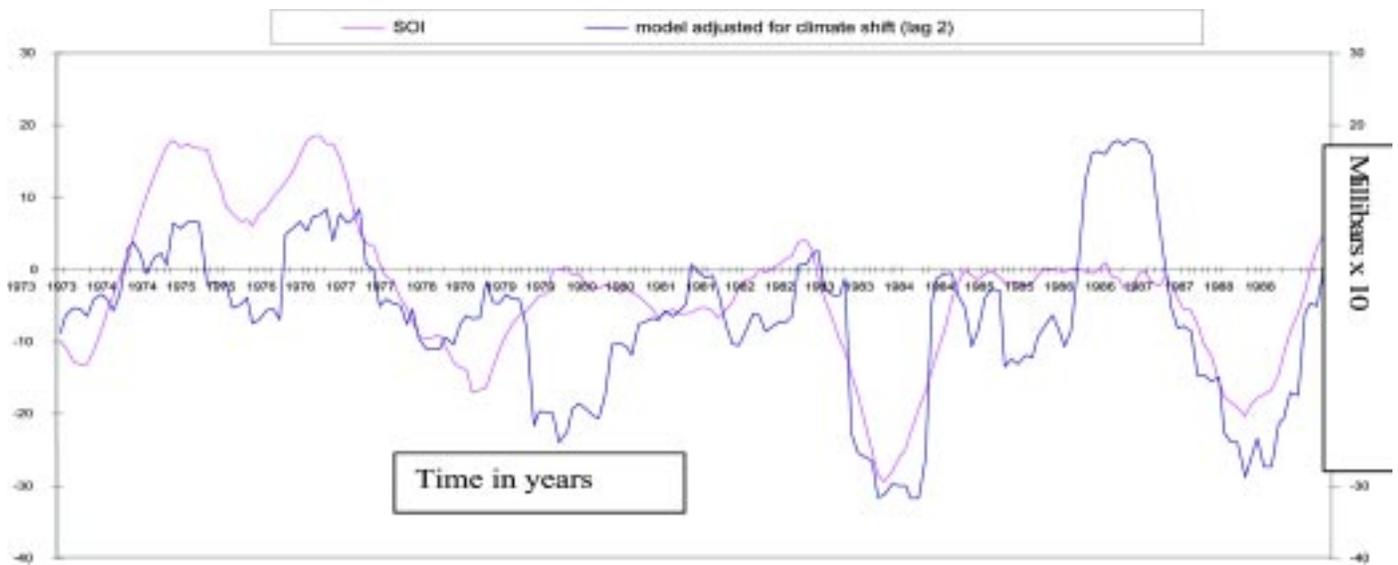


Figure 6: Model v. SOI for 1975 - 1991 after shifting the phase by 2 years to produce a fit.

CONCLUSIONS

We have a simple computer model which predicts the SOI ten years in advance. The model is based on assumptions that the conveyor is much faster than generally accepted and that changes in conveyor behavior in the Atlantic Ocean can have an immediate effect on conveyor behavior in the Pacific. These assumptions have not been proven valid and warrant more research before they can be accepted.

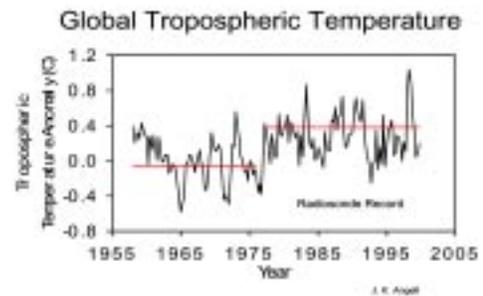


Figure 7: Global Tropospheric Temperature

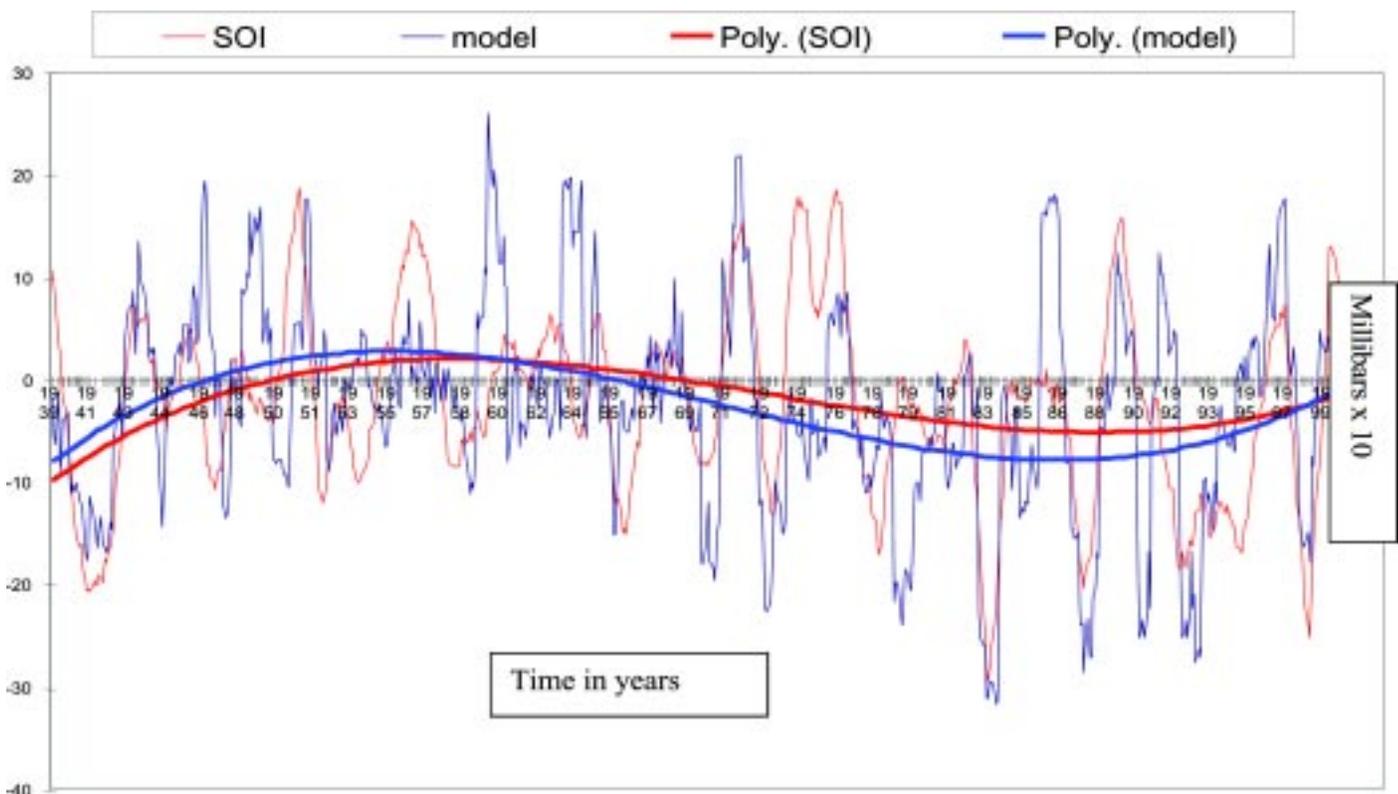


Figure 8: Final SOI Model v. SOI Actual

The model does show, if nothing else, that salt influence from the Red Sea could produce oscillations of the proper frequency as those observed in ENSO. Furthermore, the model correctly predicts long-term oscillations in the SOI that were not manually fitted. The short-term oscillations fit properly only for the time period that they were manually fitted, but the structure (i.e. width, distance between and approximate magnitude of major peaks) was also accurate for times in which the model was not manually fitted. Though the phase difference had to be manually eliminated, it is shown that the adjustment corresponds with another known climatological phenomenon. A model which incorporates changing lags due to varying conveyor speed rather than fixed lags would theoretically be more accurate.

The model actually predicts conveyor behavior, opening the possibility of its ability to predict other climatological factors with little adjustment. More research should be done to improve the SOI model itself as well as use the model to predict Atlantic hurricane seasons, global and local average temperatures and precipitation, and other global climate phenomenon.

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COMPARISON OF TWO WIRE CHAMBER TRACK RECONSTRUCTION ALGORITHMS USED IN HALL A AT JEFFERSON LAB

SEAN DOBBS AND J. O. HANSEN

ABSTRACT

The Hall A collaboration at Jefferson Lab is currently in the process of redesigning and rewriting its physics analysis software in C++, using the ROOT libraries developed at CERN, to replace the Fortran-based ESPACE analyzer. In this paper, we carry out a detailed comparison of the wire chamber tracking results of both software packages. To this end, reconstruction of target quantities from detected tracks through the Vertical Drift Chambers (VDCs) in both spectrometer arms has been recently added to the C++ analyzer, to bring it to the same level as ESPACE. A study of the differences in the outputs of both analysis programs shows that while the output of the C++ analyzer is suitable for calibrations and studies that do not require high resolution, there are still many subtle differences that need to be resolved before it is ready for a production-quality release. The problems are most likely due to different cluster matching and track fitting algorithms used by both programs for tracks through the VDCs, as well as certain corrections missing from the C++ code. These problems and some possible solutions are discussed.

INTRODUCTION

The Hall A [1] collaboration at Jefferson Laboratory [2] is currently in the process of redesigning and rewriting its physics analysis software [3] in C++ using the ROOT libraries developed at CERN [4]. This software is intended to replace ESPACE [5], the current Fortran-based analysis software used in Hall A. Major goals of the new software are increased flexibility to support a variety of new detectors planned for future hall upgrades with a minimum of extra development and the ability to handle the larger data streams these detectors would generate.

Most nuclear physics at Jefferson Lab is conducted at the Continuous Electron Beam Accelerator Facility (CEBAF). CEBAF is able to deliver a continuous beam of electrons with energies ranging from 800 MeV to 6 GeV to three different experimental halls simultaneously. Experiments in the

halls use this beam to perform detailed measurements of nuclear interactions.

Hall A uses a pair of high resolution spectrometers (HRS) with superconducting magnets to measure the charged particles scattered from the target at various angles [6]. In each spectrometer, particle tracking information is obtained using Vertical Drift Chambers (VDCs) [7]. A VDC consists of a plane of sense wires sandwiched between conducting planes that are kept at a high voltage. This creates a strong electric field in the chamber which is constant and perpendicular to the wire plane throughout most of the chamber, though near the wires it becomes approximately radial. The chamber is filled with a gas that is easily ionized as charged particles pass through it. The electrons liberated from the gas when ionized drift towards the wires along the electric field lines at a nearly constant velocity. As these electrons drift into the region of very strong electrical field near the wires, they acquire enough energy to ionize other gas molecules, creating

an avalanche effect that greatly increases the number of ionized atoms generated by a particle track. The drift of the electrons towards the sense wires and that of the ions in the other direction induces a current in the sense wires, so the avalanche effect creates a signal that is easily measured with standard electronics [9, 10].

Each HRS arm contains two pairs of VDCs. The two VDCs of each pair are labelled U and V. The separation between like pairs of VDC planes is 332.7mm for the left arm and 334.8mm for the right arm. Each VDC contains 368 sense wires, and the wire spacing and vertical extent of the chambers give a cell width of 4.24mm and a cell height of 26mm for each sense wire. The VDCs are filled with a gas mixture of 62% argon to 38% ethane and are operated at a voltage of 4.0kV. The VDCs are oriented horizontally in the laboratory frame, so that the central angle that tracks take through the VDCs is 45°. This means that a particle on its way through a VDC plane will travel through on average five cells. The sense wires for the U and V planes lie orthogonal to each other and 45° to the main axes of the HRS [8, 13]. Several coordinate

Next, in the VDC analysis, a series of consecutive wires with induced signals, called a cluster, is identified. Each cluster usually corresponds to a single track. The drift times for each hit in a cluster are typically converted to drift distances, and a linear fit is performed on these distances to determine the local cross-over point in the plane and the local angle of the track. However, the relation between drift time and perpendicular drift distance is not quite linear, in part because of radial nature of the field lines near the sense wires, which increases the proportion of events with short times, and also from the fact that some tracks leave the VDC plane before they leave the wire cell, which can produce excessively long drift times [10]. These aberrations are corrected by the analysis software.

The algorithms used by both ESPACE and the C++ analyzer to calculate quantities in the detector coordinate system differ slightly. ESPACE uses pairs of calculated cross-over points in the U and V planes to calculate the directions of the path in a coordinate system defined by the U and V planes. This system is rotated 45° around the z-axis from the detector coordinates, so ESPACE must then

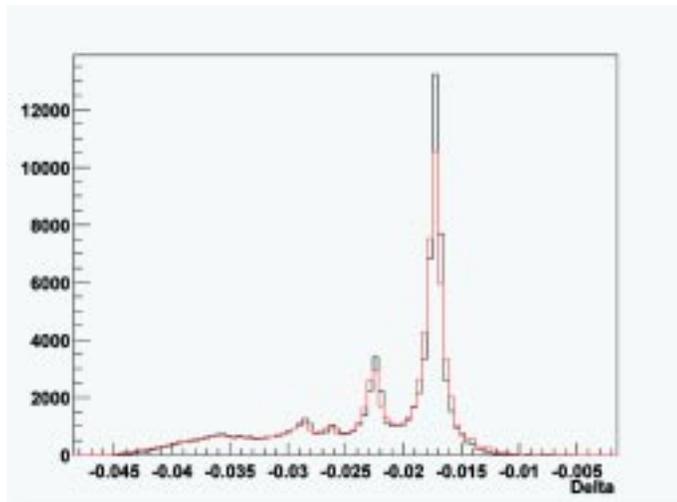


Figure 1: Right arm δ spectrum.

systems are used in the reconstruction algorithm. The reader interested in the exact definition of these systems is directed to references [8, 12] for a detailed discussion.

The basic algorithm for particle tracking in a VDC is straightforward. First, the so-called drift times are measured, that is, the time elapsed between the initial ionization in the sensing range of a wire and the creation of a signal in the wire. The time measurement is done with a time-to-digital converter (TDC) in “common-stop” mode, where the common stop signal is given by the delayed event trigger produced by the data acquisition unit, and the TDCs are started with the amplified and discriminated signals from the sense wires. Thus, higher TDC values correspond to shorter drift times.

$$y_{ig} = \sum_{i,j,k,l} C_{ijkl}^y x_{fp}^i \theta_{fp}^j y_{fp}^k \phi_{fp}^l \quad (1)$$

$$\theta_{ig} = \sum_{i,j,k,l} C_{ijkl}^T x_{fp}^i \theta_{fp}^j y_{fp}^k \phi_{fp}^l \quad (2)$$

$$\phi_{ig} = \sum_{i,j,k,l} C_{ijkl}^P x_{fp}^i \theta_{fp}^j y_{fp}^k \phi_{fp}^l \quad (3)$$

$$\delta = \sum_{i,j,k,l} C_{ijkl}^D x_{fp}^i \theta_{fp}^j y_{fp}^k \phi_{fp}^l \quad (4)$$

perform a further transformation to get the detector coordinates. The C++ analyzer, however, uses each related pair of U and V plane clusters to form a local cross-over point and direction using input from the cluster fitting procedure. These local directions are then used to match up clusters from the first VDC pair to similar clusters in the second VDC pair, from which the global track is calculated in detector coordinates. This algorithm was chosen because it was more natural to the object-oriented design used in the C++ analyzer.

Both programs then convert detector coordinates into focal plane coordinates. Focal plane coordinates are defined in a so-called “rotating” reference frame. This frame is defined by a rotation of the detector coordinate system about the y-axis such that the z-axis points along the *local* central angle at a given point in the focal plane. The rotation angle is roughly 45°, but varies due to the spectrometer’s dispersion.

Focal plane coordinates present favorable numerical characteristics for target reconstruction as θ is always minimized. A set of zeroth-order matrix elements, such as those described in the following paragraphs, are used in the conversion to help approximate the local central angle [12].

After the particle tracks at the VDCs are computed at the focal plane, that information can be used to reconstruct the corresponding quantities at the target. From the focal plane, the transformation of the measured quantities through the magnetic elements of the spectrometer can be calculated using a technique similar to the TRANSPORT formalism [11].

For target reconstruction through the spectrometer, there are five coordinates to consider: the displacement and angular deviation in the dispersive direction, x and θ ; the displacement and angular deviation in the non-dispersive direction, y and δ ; and the fractional momentum difference, δ , which is defined as $p/p_0 - 1$, where p is the particle's momentum and p_0 is the central momentum of the detector. Since the VDCs only detect four quantities, x , y , θ , and δ , mathematically we can only reconstruct four quantities at the target. We choose those with the most physical relevance: y , θ , ϕ , and δ . x_{tg} is normally defined by the vertical beam position and can be measured independently. y_{tg} is essentially the interaction position along the beam. θ_{tg} and δ_{tg} are the in-plane and out-of-plane scattering angles respectively.

The focal plane coordinates are linked to the target coordinates by the Transport Tensor as follows: where C_{ijkl} are the coefficients describing the various matrix elements. In practice, the matrix elements are stored up to fifth order. The matrix elements are numerically calculated through a series of calibration experiments by fitting experimental data, and are then stored for later use [12].

The target coordinates can now be used to determine the physics of the experiment. The goal of this paper is to study differences between the results given by ESPACE and the C++ analyzer at the detector coordinate level and also at the very important target level. The next section will discuss the data and analysis techniques used. The section following that will present some of the more important differences between ESPACE and the new analyzer. The final section will discuss these differences in more detail and their implications. Areas of investigation and potential further improvements to the C++ analyzer will also be presented.

METHODS

The data used for this study is from an optics commissioning run (run number 1146 [14]) for Hall A experiment E97-111, taken on September 30, 2000. A sieve slit was installed in the spectrometer, in conjunction with a target consisting of nine thin ^{12}C foils placed 4cm apart. This setup is typical for collecting data to be used in optics calibrations. The in-

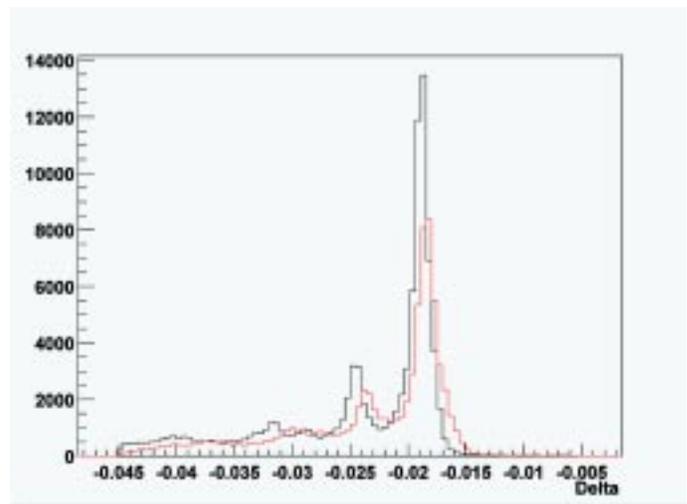


Figure 2: Left arm δ spectrum.

coming electron beam was at an energy of 825 MeV. The right spectrometer arm was set to an angle of 16.009° with a central momentum of 837.00 MeV. The left arm was set to an angle of 15.965° with a central momentum also of 837.00 MeV.

As part of this project, the target reconstruction algorithm as described in the previous section (eqs. 1-4) was implemented in the C++ analyzer. The first 200,000 physics events were run through both analysis programs and their

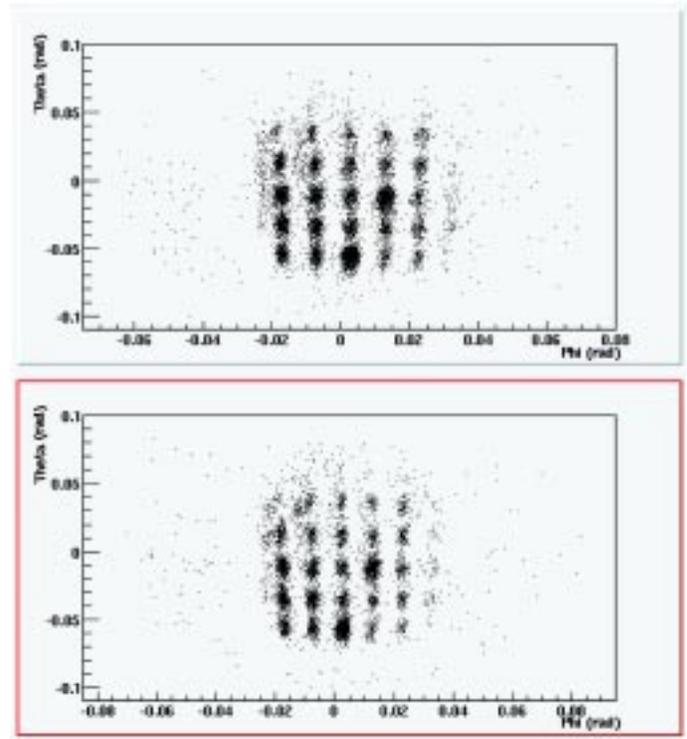


Figure 3: A plot of θ_{tg} against ϕ_{tg} for the left arm for tracks using a cut of $9.5\text{mm} < y_{tg} < 15.5\text{mm}$ to pick out one foil. The top graph is generated by the C++ analyzer, while the bottom graph is generated with ESPACE.

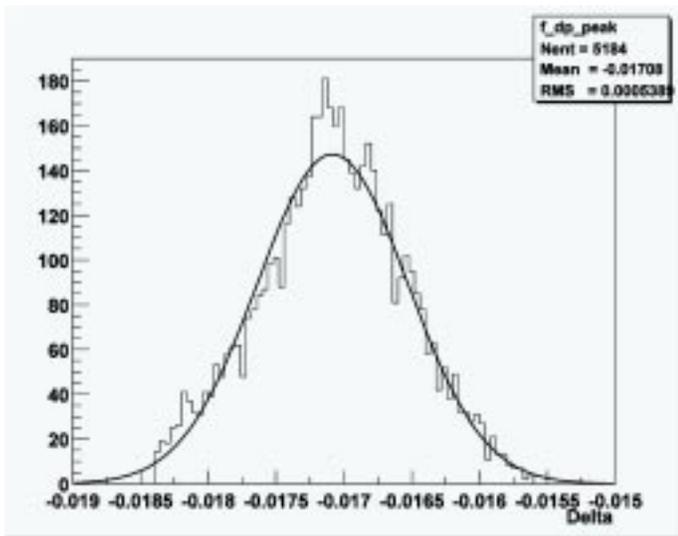


Figure 4: The elastic peak in the right arm ESPACE δ spectrum with kinematic corrections added. A gaussian curve has been fit to the peak.

output was compared. The matrix elements used for both programs are calibrated for analysis with ESPACE and have been found to be stable for analysis with that program [12].

The main analysis was performed on a PIII 700Mhz Dell PC, with 768 MB of RAM, running Red Hat Linux 7.2. ESPACE version 2.9.2 was used along with a development version of the ROOT/C++ analyzer based on version 0.65.

RESULTS

We only show selected results in this paper. Many areas were studied, including simple comparisons between ESPACE and C++ analyzer values, correlations between related values, such as x_{tp} and y_{tp} or x_{tp} and θ_{tp} , and event-by-

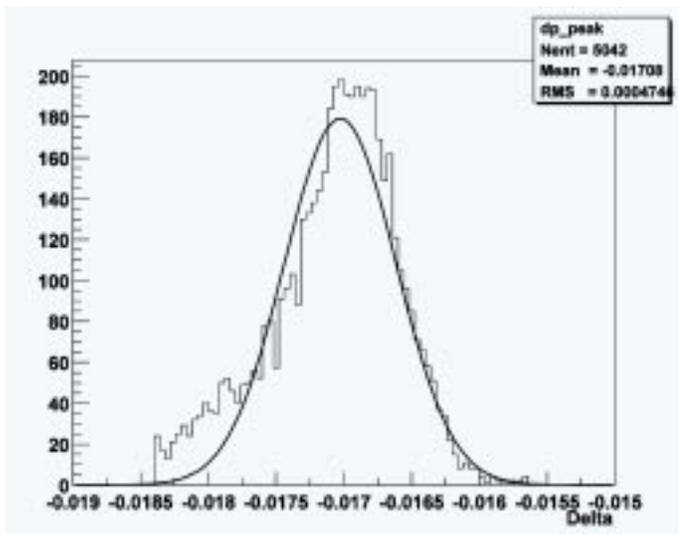


Figure 5: The elastic peak in the right arm C++ analyzer δ spectrum with kinematic corrections added. A gaussian curve has been fit to the peak.

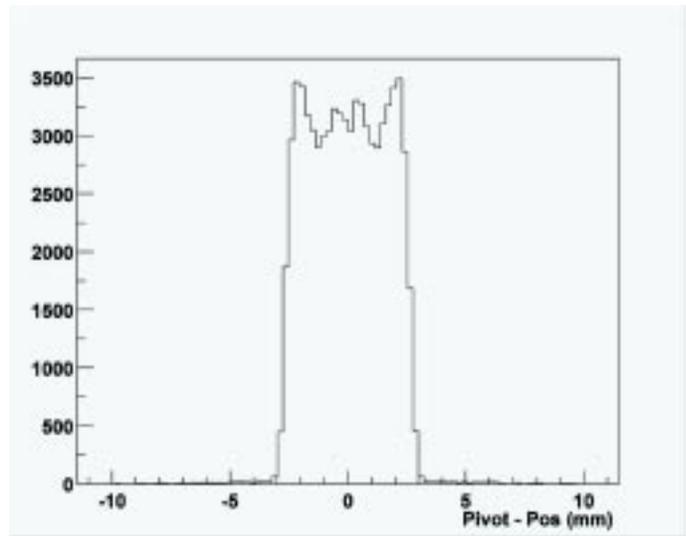


Figure 6: The difference in the cluster pivot wire and the crossing-over point for a track in the U1 VDC plane in the left arm as determined by ESPACE.

event cross-correlations and differences between ESPACE and the C++ analyzer.

Tables 1 and 2 give the results of an analysis of the difference in target values as calculated by ESPACE and the C++ analyzer for both HRS arms. Table 3 gives the results of a similar analysis for values at the focal plane. The differences were calculated on an event-by-event basis. The resulting distributions are essentially gaussian, except for x_{tp} and θ_{tp} on both arms, and θ_{tg} and δ on the left arm, which all have sizeable tails. Figures 1 and 2 give the δ spectrum for the right and left arm respectively. In all such graphs, the ESPACE results are given by the light-colored lines.

The tall peak in the δ spectrum is known as the elastic peak, as it results from elastic scattering of electrons from

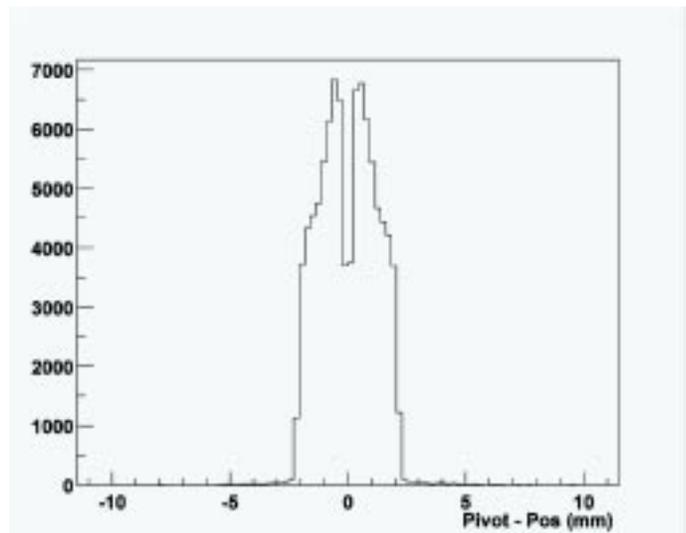


Figure 7: The difference in the cluster pivot wire and the crossing-over point for a track in the U1 VDC plane in the left arm as determined by the C++ analyzer.

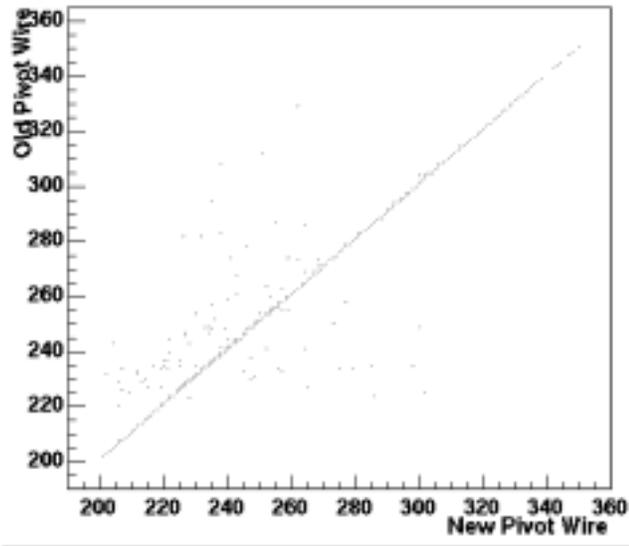


Figure 8: A plot of the cluster pivot wire for the U1 VDC plane in the left arm as determined by ESPACE against the pivot wire determined by the new C++ analyzer.

the ^{12}C nucleus. It is theoretically infinitesimally small, but its finite width is due to spectrometer resolution and radiative effects. The Δ resolution was estimated by fitting a gaussian curve to this peak, after corrections for kinematical broadening were applied. No radiative correction was made, so the estimated resolution is worse than the actual value. The peak was taken to range from a Δ value of 0.0156 to 0.00184. Figures 3 and 4 show the result of these curve fits for the right arm.

Figure 5 gives a comparison of a plot of \hat{e}_{ig} against \hat{a}_{ig} for tracks using a cut of $9.5\text{mm} < y_{ig} < 15.5\text{mm}$ to pick out one foil for both ESPACE and the C++ analyzer. The sieve slit pattern is clearly visible in this graph, indicating that the target reconstruction is essentially working in the C++ analyzer and agrees substantially with the results from ESPACE.

Figures 6 and 7 give a plot of the difference between the pivot wire position and calculated cross-over position for clusters in the U1 VDC plane of the left arm. Figure 8 gives a cross-correlation plot of the pivot wire number for clusters in

	Mean Difference	RMS	Optics Comm.	Design Target
Left arm y_{ig}	-0.3 mm	3.1 mm	4.0 mm	1.5 mm
Right arm y_{ig}	-0.4 mm	2.5 mm		
Left arm θ_{ig}	-1.7 mrad	7.9 mrad	6.0 mrad	2.0 mrad
Right arm θ_{ig}	-0.9 mrad	5.4 mrad		
Left arm ϕ_{ig}	0.2 mrad	1.6 mrad	2.0 mrad	0.6 mrad
Right arm ϕ_{ig}	-0.5 mrad	1.3 mrad		

Table 1. The differences in reconstructed target values between ESPACE and the C++ analyzer were calculated for each arm and a gaussian curve was fit to each difference. Given are the mean and RMS values for each distribution. For comparison to the RMS, the resolutions obtained at optics commissioning and the maximum design values for the HRS are given (both FWHM).

	Elastic Peak	RMS	Optics Comm.	Design Target
Left arm δ_{ESPACE}	-0.018589	0.000299	0.000250	0.000100
Left arm $\delta_{\text{C++}}$	-0.019009	0.000315		
Right arm δ_{ESPACE}	-0.017079	0.000539		
Right arm $\delta_{\text{C++}}$	-0.017076	0.000475		

Table 2. The location and RMS width of the elastic peak seen in ^{12}C scattering in the Δ spectrum in both arms for both ESPACE and the C++ analyzer. The locations of the peaks are different in each arm due to the different positioning of the arms. For comparison to the RMS, the resolutions obtained at optics commissioning and the maximum design values for the HRS are given (both FWHM).

the U1 left arm VDC plane between ESPACE and the C++ analyzer. The line is slightly inclined due to a trivial difference in numbering between Fortran and C++. For these plots, only clusters belonging to tracks that produced one cluster in all 4 VDC planes were chosen.

CONCLUSIONS

As can be seen from Tables 1 and 2, the deviations of the results obtained using the C++ analyzer from those obtained with ESPACE are almost all well within the error of their distributions. Ideally, the distributions of these differences between the analyzers should be delta functions, showing no difference. However, the C++ analyzer does not include some of the corrections that ESPACE does, such as corrections for time-of-flight between the VDCs and the trigger scintillator, which should lead to purely statistical fluctuations, yielding a gaussian peak. Indeed, for nearly every variable, we find this to be the case. The resolutions of the target values are on the same order as those calculated with ESPACE during detector commissioning, so they seem to be quite reasonable. This suggests that the C++ analyzer is ready to be used for basic analysis that does not require very high resolution.

However, there are still some lingering problems. Looking at Table 1, we see that the left arm \hat{e}_{ig} has by far the largest deviation and an unusually large distribution. The main cause of this can be traced back to deviations in the related values x_{fp} and \hat{e}_{fp} , given in Table 3. \hat{e}_{fp} does not have a very large deviation, however, \hat{e}_{ig} has a complicated dependence

	Mean Difference	RMS		Mean Difference	RMS
Left arm x_t	-0.7 mm	0.7 mm	Left arm x_{fp}	-0.7 mm	0.7 mm
Right arm x_t	0.5 mm	0.8 mm	Right arm x_{fp}	0.5 mm	0.3 mm
Left arm y_t	-0.3 mm	0.7 mm	Left arm y_{fp}	-0.3 mm	0.7 mm
Right arm y_t	0.6 mm	0.9 mm	Right arm y_{fp}	0.9 mm	0.3 mm
Left arm θ_t	-1.5 mrad	1.9 mrad	Left arm θ_{fp}	0.8 mrad	3.1 mrad
Right arm θ_t	-0.3 mrad	1.2 mrad	Right arm θ_{fp}	-0.5 mrad	0.8 mrad
Left arm ϕ_t	0.02 mrad	2.1 mrad	Left arm ϕ_{fp}	0.04 mrad	2.1 mrad
Right arm ϕ_t	-0.3 mrad	1.2 mrad	Right arm ϕ_{fp}	0.2 mrad	0.9 mrad

Table 3. The differences in reconstructed focal plan values between ESPACE and the C++ analyzer were calculated for each arm and a gaussian curve was fit to each difference. Given are the mean and RMS values for each distribution. The t subscript signifies values in the standard Transport coordinate system at the focal plane, while the fp subscript signifies values at the focal plane in the rotating coordinate system.

on θ_{fp} , which through the Transport Tensor can consist of a number of high-order polynomials. Also, the deviations in x_{fp} can cause inaccuracies in the reconstruction procedure, since the polynomials used depend on powers of x_{fp} . Such dependences could easily explain the unusual distribution for θ_{fp} in the left arm and can lead to larger errors than would otherwise be expected.

Another unusual effect can be seen by comparing Figures 1 and 3. The distributions for the right arm match up well, whereas the peaks in the left arm are shifted to negative energies by an amount that appears to depend on the value of δ . As δ also has a similar complicated dependence on θ_{fp} and x_{fp} , the slight difference noted above could easily explain the distorted peaks. The cause of these shifts in θ_{fp} and x_{fp} are currently not well understood, but a possible cause is mentioned below.

Another problematic effect can be seen in Figure 3. The holes in the sieve slit form a grid of straight lines, and this should be readily apparent in the given plot. However, the lines from the C++ analyzer in the top plot show slight diversions with increasing θ_{fp} , unlike the ESPACE results on the bottom. This effect is likely related to the above-mentioned errors in focal-plane quantities, but it is very minor, and overall this figure is a prime example of the C++ analyzer's readiness for use.

An interesting difference is seen when the elastic peaks measured in the right arm with both programs are compared. Both programs give a value for the center of the peak that agrees within 3 keV (0.001%). However, The ESPACE results, shown in Figure 4, give a broad, nearly gaussian peak. The C++ analyzer, as shown in Figure 5, gives a narrower peak, but one that has a distinct tail. This could be the radiative tail of the elastic peak, or an inaccuracy in the C++ analyzer algorithm. Modeling of the expected radiative tail would help clarify the source of this difference.

A potential low-level problem in the VDC tracking algorithm of the C++ analyzer is suggested by looking at the differences in the pivot wire position and the calculated cross-over position for both ESPACE, shown in Figure 6, and the C++ analyzer, shown in Figure 7. The cross-over point is calculated by fitting the drift distances in the cluster to a line, which is done after cluster identification. Since the density of tracks in a wire cell is approximately constant, this spectrum of distance variation should be close to flat, as it is with ESPACE. However, the C++ analyzer produces a highly structured spectrum. The reasons for this are not completely known, but could come from incorrectly calculated drift times, non-linearities in the drift spectrum, or errors in the fitting code. The cross-over positions are used to calculate locations in the focal plane, so errors in their calculation could be the cause of the deviations in x_{fp} . Also, since the angles of the tracks are highly dependent on the cross-over positions calculated in this way, these errors might be the cause of the shift in θ_{fp} that was discussed above.

Figure 8 points to two related problems in the cluster identifying algorithm. Because this graph looks simply at the pivot wires of clusters, it does not depend on such compli-

cated line-fitting functions as are used later in analysis, and therefore the line should be very nearly straight. However, while most clusters belong to only one track, if two tracks get close enough to each other, their clusters overlap. This explains some of the variation, as ESPACE handles this case, but the C++ analyzer as yet does not. However, since the average size of a cluster is only five wires, this explanation only works for those wires within a certain range of the pivot. There are some differences in this plot that are much larger, which are most likely due to some misidentification of the clusters.

Besides the above-mentioned problems that need to be investigated, there are a few other improvements that could be made to increase the accuracy of the C++ analyzer. The event trigger that stops the TDCs is derived from scintillator signals. This introduces some slight inaccuracies, which ESPACE corrects for, but the C++ analyzer does not. A correction can also be added for the timewalk of the scintillator timing. Also, effective cluster reconstruction algorithms, for tracks that do not create clusters in each plane, can improve analysis efficiency.

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Fred Schlachter is a staff scientist at the Advanced Light Source, Lawrence Berkeley National Lab. He received his education in physics at the University of California in Berkeley and the University of Wisconsin in Madison. He worked for several years in France at Saclay and the University of Paris. Fred has done research in atomic and molecular physics at Berkeley Lab for the past 25 years, most recently studying quantum chaos, molecular fragmentation, and photoionization of ionized matter. Alongside his research publications is an article in Scientific American on ultrabright synchrotron light sources.

PHOTOIONIZATION OF Fe^{3+} IONS

OLGA OVCHINNIKOV AND FRED SCHLACHTER

ABSTRACT

Photoionization of Fe^{3+} ions was studied for the first time using synchrotron radiation from the Advanced Light Source (ALS) and the merged-beams technique. Fe^{3+} ions were successfully produced using ferrocene in an electron cyclotron resonance ion source (ECR). The measured yield of Fe^{4+} photoions as a function of photon energy revealed the presence of resonances that correspond to excitation of autoionizing states. These resonances are superimposed upon the photoion yield produced by direct photoionization, which is a smooth, slowly decreasing function of energy. The spectra for the photoionization of Fe^{3+} will be analyzed and compared with theory. The data collected will also serve to test models for the propagation of light through ionized matter.

INTRODUCTION

Almost all the information we receive about our universe comes from light from distant stars, and more than 99% of the matter in the universe is found in ionized form. Therefore studies of photoionization of ions provide data for the modeling of propagation of light through space, which is critical for our understanding of the universe. The photoionization of ions is the removal of one or more electrons by absorbing energy from light radiation (photons). In our experiment one-electron photoionization of ions was observed.

Iron is a common element not only on earth but also in the universe. In interstellar space, iron mainly exists in ionized form and can readily undergo photoionization by the radiation of stars, quasars, and other astronomical occurrences. Therefore the light that we receive could be affected by photoionization and thus it is necessary to study and understand the photoionization process of ions.

A third-generation synchrotron light source contains insertion devices called undulators that create photon beams in a narrow energy and angular range, producing an intense, nearly parallel light beam. Using the synchrotron radiation from the third-generation Advanced Light Source (ALS) and the merged-beams technique (Covington et al 2002) it was

possible to observe the photoionization of Fe^{3+} for the first time.

There are two mechanisms of photoionization of Fe^{3+} . One is direct photoionization that serves as a background, rising from zero as a step function at the ionization energy threshold and falling smoothly with increasing photon energy (Figure 1),

The second is the indirect process and is characterized by excitation of Fe^{3+} to a doubly excited intermediate state that decays spontaneously by a process called autoionization, ejecting an electron:

This process gives rise to resonances occurring at varying photon energies that correspond to the excitation of autoionizing states. Interference between the direct and indirect photoionization pathways yields asymmetric resonance line shapes.

Measurement of these processes is crucial to our understanding of the universe. However until recently it was very difficult to obtain experimental data on these phenom-

PHOTOIONIZATION MECHANISMS

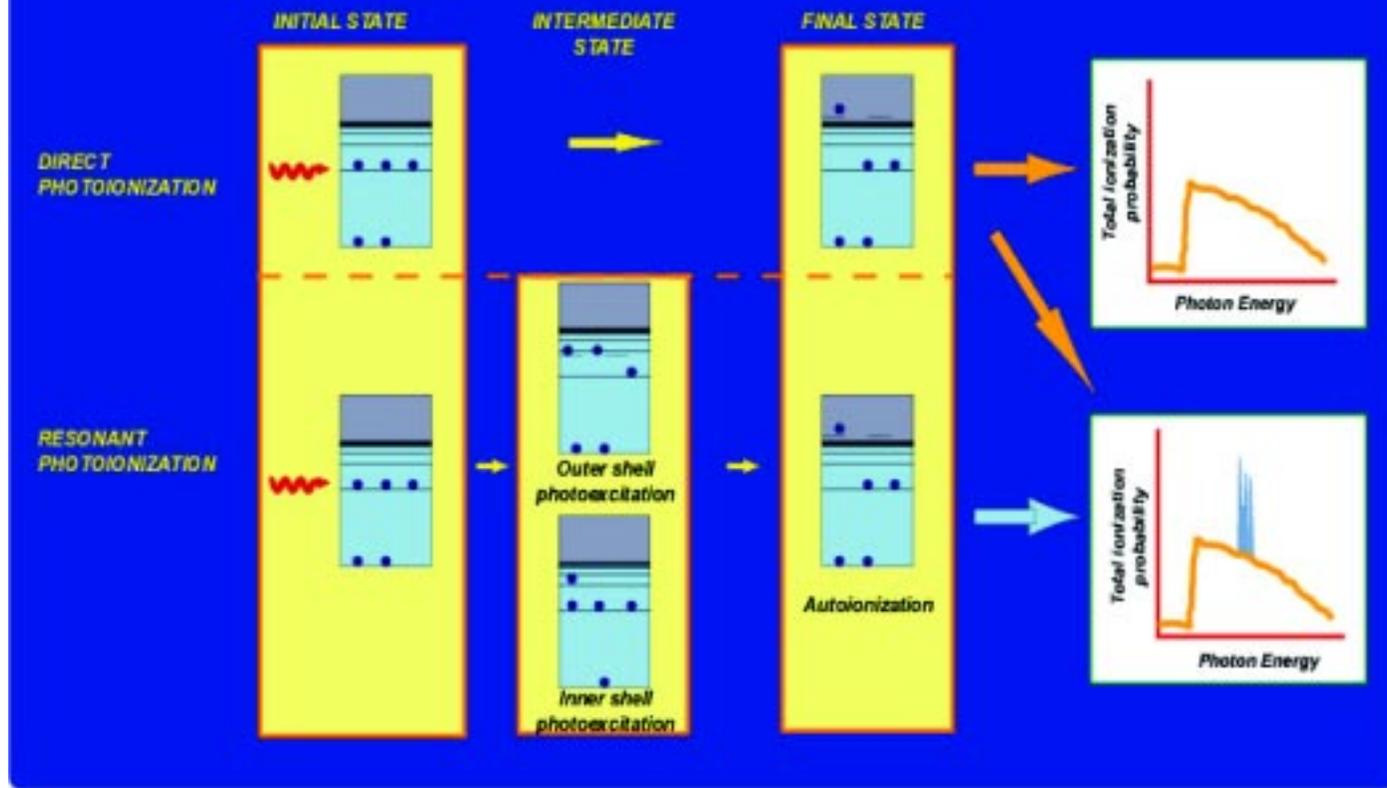


Figure 1: Diagram for the photoionization process. As may be seen from the diagram there are two processes involved in photoionization. The direct process creates the smooth background while the indirect process is responsible for the resonance structure observed in photoionization.

ena due to the technical difficulty of producing ion and photon beam of sufficient density. These problems have been largely overcome by combining third-generation synchrotron radiation sources and the merged-beams technique.

METHODS

The photoionization measurements were based on the merged-beams technique. The photon beam was produced by an undulator at the ALS Beamline 10.0.1 (Figure 2). A grazing incidence monochromator selected a collimated photon beam with a radius of less than 0.5 mm and a flux of up to 10^{13} photons/second over an energy range of 17-340 eV. The spectral resolution of the light exiting the monochromator was selected by adjusting the entrance and exit slits (Figure 2). The photon beam was chopped, which separated photoions from other ions created by interactions with residual gas in the merged path. The flux of the photons was measured by a silicon X-ray photodiode in the beamline, for which the average value was found to be $2-3 \times 10^{13}$ photons/second. The current of the photodiode was directed to a current amplifier, whose analog output was sent to a voltage-

to-frequency converter, which provided counts to a scaler in the data acquisition computer.

The Fe^{3+} target ions were produced by the evaporation of ferrocene, which was directed in gaseous form to an all permanent-magnet electron cyclotron resonance ion source (ECR) (Müller et al 2002). The ion beam was accelerated through a potential difference of 6 kV, focused and directed using a series of cylindrical electrostatic einzel lenses and steering plates (Figure 3). The cross-sectional area was defined by adjusting vertical and horizontal beam-defining slits located downstream of the analyzing magnet.

The 18 keV Fe^{3+} ion beam was merged onto the counter-propagating photon beam using a 90° spherical-sector electrostatic deflector. The spatial overlap of the ion and photon beams was optimized by the use of two sets of perpendicular electrostatic steering plates located before the merger plates. The interaction region is defined by a stainless-steel-mesh cylinder whose entrance and exit apertures are separated by 29.4 cm. In order to energy-label the photoions produced inside the interaction region, an electrical potential of +1.7 kV was applied. The two-dimensional overlap of both beams was observed by rotating-wire beam profile monitors located directly before and after the interaction region and a scanning slit located in the interaction region (Figure 4).

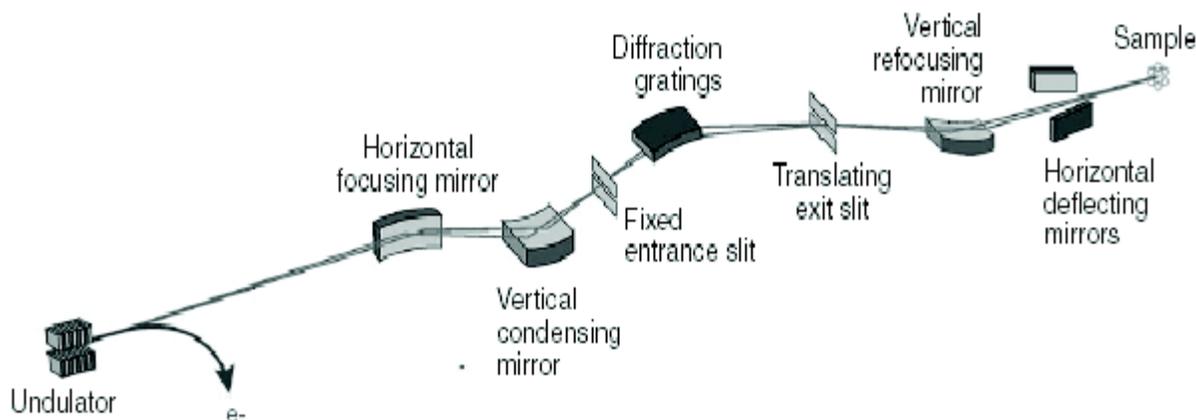


Figure 2: Schematic layout of ALS beamline 10.0.1 optics.

The Fe^{4+} photoionization products were separated from the parent Fe^{3+} beam by a 45° dipole-analyzing magnet located after the interaction region (Figure 3). The parent Fe^{3+} beam was collected in an extended Faraday cup connected to a current amplifier, whose analog output was sent to a voltage-to-frequency converter, which provided counts to a scaler in the data acquisition computer.

The Fe^{4+} products were directed through a small opening at the top of the Faraday cup to a 90° spherical electrostatic deflector, and onto a stainless steel plate biased to -550 V. The secondary electrons produced by the collision of Fe^{4+} ions with the stainless steel plate were directed to a microchannel-plate detector, which generated an electrical pulse for each Fe^{4+} ion. This pulse was sent to an amplifier followed by a single-channel analyzer, which set a threshold level to reject background electronic noise. The signal pulses were sent to a scaler in the data acquisition computer.

RESULTS

Using the merged-beam technique and synchrotron radiation, the photoion yield of Fe^{4+} was measured at a constant resolution of 40 meV from 43.5 to 62.5 eV. These data were taken with step sizes of 4 meV (Figure 5). The spectrum is divided into 3 different energy regions. The first region, 43.5 to 50 eV, shows three resonances with decaying intensities implying the presence of a Rydberg series (Figure 5). Further analysis complemented with atomic structure calculations will be needed in order to identify the nature of these resonances. The second energy range, from 50 to 55.5 eV, is primarily dominated by the direct photoionization process, although the presence of weak structure can be distinguished (Figure 5). Finally, the last section of data from 55.5 to 62.5 eV shows a dramatic increase in the

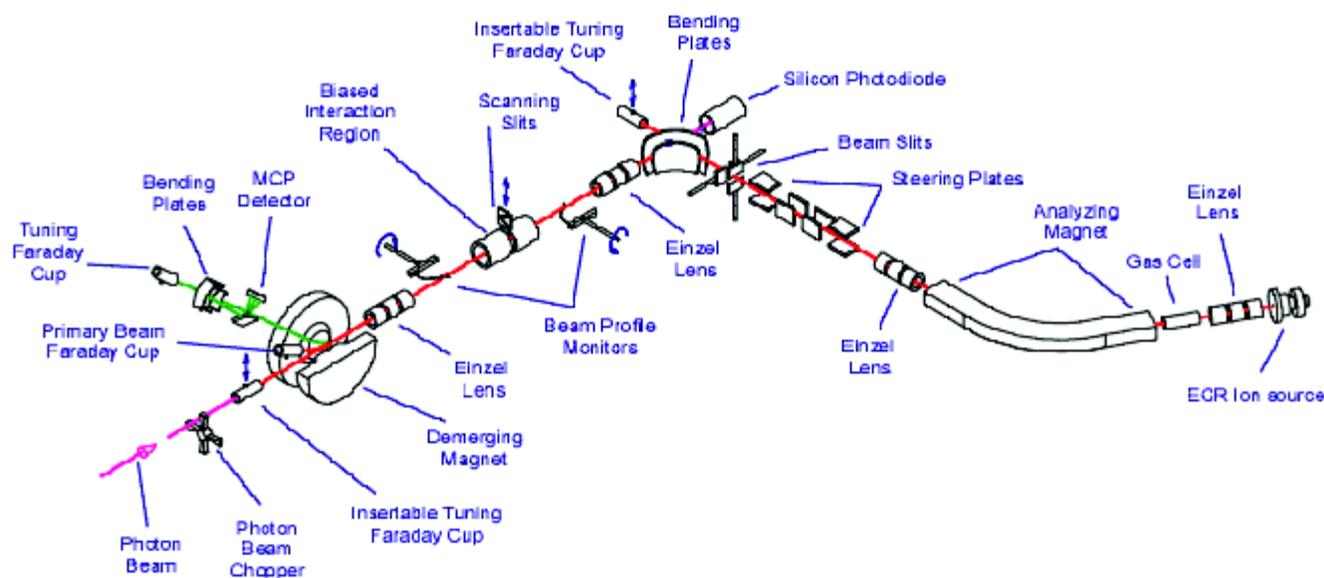


Figure 3: Ion Photon Beam (IPB) endstation installed at the ALS beamline 10.0.1

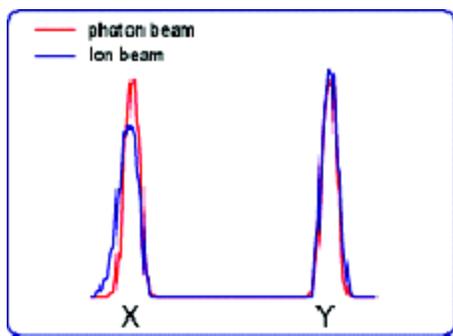


Figure 4: Two-dimensional spatial overlap profile of a photon and an ion beam.

photoion yield starting at 56 eV (Figure 5). Such increases of the photoion yields are common in the photoionization of positive ions when new channels open or thresholds for metastable species are reached. However, in this case the slope of increase of photoion yield is very smooth and gradual with energy, compared to the abrupt rise expected at a threshold. Furthermore, the photoion yield begins to decrease at 61 eV, suggesting the presence of an extremely broad resonance, corresponding to creation of a short-lived state that decays rapidly by the process of autoionization.

This experiment demonstrated the feasibility of studying

experimentally the photoionization of an astrophysically abundant multiply charged metallic element like iron, whose photoionization spectrum had not previously been observed.

DISCUSSION

In this experiment the use of synchrotron radiation and the merged-beams technique allowed the observation of Fe^{4+} photoions for the first time. The experiment is an important step in photoionization studies, because until recently the technical difficulties of producing well-characterized multicharged ion and photon targets of sufficient density impeded the study of photoionization of highly charged ions. These difficulties have now been overcome by combining a merged-beams apparatus, an electron-cyclotron-resonance (ECR) multicharged ion source and a third-generation synchrotron radiation source, at the 10.0.1 undulator beamline at the Advanced Light Source (ALS).

The results obtained in the experiment indicate that it is possible to produce Fe^{3+} ions using the evaporation of ferrocene ($\text{C}_{10}\text{H}_{10}\text{Fe}$) and the ECR source. The experiment demonstrated that it is possible to photoionize the Fe^{3+} ions to

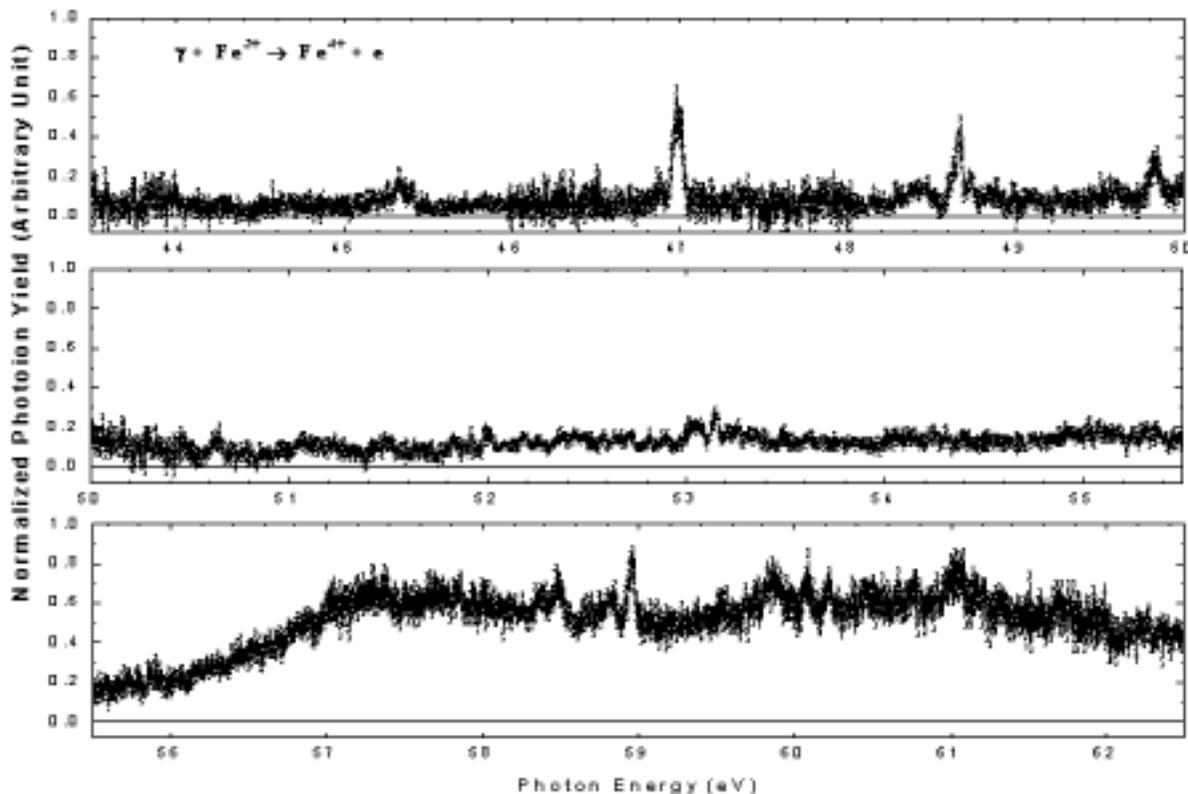


Figure 5: Graph of data collected on photoionization of Fe^{3+} .

create Fe^{4+} ions and to detect the photoions. The measurements of the relative yield of Fe^{4+} photoions as a function of the photon beam energy revealed the presence of resonance structures at certain energies. The energy positions and relative magnitudes of these resonance structures observed will serve as benchmarks for theory. Further photoionization studies of Fe^{3+} that are planned will place the present measurements on an absolute cross-section scale. These studies will also examine in depth each energy range where a resonance is present, and also the energy range of the ionization threshold (ionization potential). Such data will then be used to model various astrophysical phenomena like the propagation of light through the atmospheres of stars. They will also be helpful in interpreting light emissions from laboratory plasmas and from reactors that are being developed to extract energy from thermonuclear fusion reactions.

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METASTABLE KRYPTON BEAM SOURCE VIA TWO-PHOTON PUMPING TECHNIQUE

WILLIE WAI-YEUNG WONG AND LINDA YOUNG

ABSTRACT

Metastable beams of rare gas atoms have wide applications in chemical analysis of samples, as well as in aiding understanding of fundamental processes and physical attributes. Most current sources of metastable rare gas atomic beams, however, are limited in their flux density, which greatly reduces their utility in applications such as low level trace analysis and precision measurements. Previous work has demonstrated feasibility of metastable krypton production via two-photon pumping, and this paper extends that possibility into beam form. Further optimization on this scheme, moreover, promises 100-fold increase of metastable krypton flux density over that of an rf-driven discharge.

INTRODUCTION

Metastable beams of rare gas atoms have a wide range of applications in atom lithography (Berggren, Bard, & al., 1995), cold collision physics (Walhout, Sterr, Orzel, Hoogerland, & Rolston, 1995), and rare isotope detection (Chen et al., 1999). Its use in trace analysis (Chen et al., 1999) is especially promising in identification of samples both chronologically and geologically. Moreover, the same technique can be applied to chemical "branding" of objects with inert substances. Whereas the substance will not react with the object, the high internal energy of the metastable state, once achieved, enables easy detection (Chen et al., 1999). In previous studies, the metastable beams were extracted from the excitation products of a DC (Lu, Hoogerland, Milic, Baldwin, & Buckman, 2001) or rf (Chen et al., 2001) discharge, with a metastable fraction of less than 0.1%. For many applications, especially that of trace analysis, it is desirable to increase the metastable fraction to achieve higher efficiencies (Chen et al., 2001).

In this paper we extend a previously explored optical method (Young, Yang, & Dunford, 2002) to produce a beam of metastable krypton. The metastable atoms, denoted Kr^* ,

are of the 5s, $J=2$ metastable state. Contrasted to the previous electron based methods, which are non-discriminatory between different excitation states, the specifically targeted photons produce a higher fraction of the desired Kr^* . Because of its odd parity and $J=2$ angular momentum state, three E1 photons are needed to arrive at the Kr^* state from the even, $J=0$ ground state (Young et al., 2002). Here we use the same excitation pathway as the Young et al. (2002) paper, namely resonant two-photon excitation at 124 nm and 819 nm, with an ensuing 760 nm decay.

MATERIALS AND METHODS

The basic design for the experiment can be seen in figures 1 and 2. The apparatus consists of two stainless-steel vacuum chambers. The first one is the production chamber, and the second one the probe. The two figures represent, respectively, the processes in each of the chambers. A beam of krypton is produced in the primary production chamber by drawing a vacuum in the production chamber and letting in krypton gas through a capillary array affixed to the end of a guiding tube. With a turbo-molecular pump running on the production chamber, we can maintain a steady pressure of

4 mTorr in the chamber with an inlet pressure of 7 Torr. The two values vary approximately linearly in the high pressure regime (2 mTorr and above) and the chamber pressure decreases more rapidly than the inlet pressure in low pressures (up to 1 mTorr). The capillary array has an aspect ratio of one to forty, thereby restricting the angular divergence of the atomic beam to 5×10^{-4} sr. By constricting the aperture of the capillary array to 5 mm, we ensured the beam's ability to traverse the distance between the two chambers (approximately 25 cm) without interacting with the walls of the conducting tubes (approximately 7 cm in diameter). The Kr^* is induced in the krypton gas through resonant optical pumping.

As seen in figures 1 and 3, we introduce the ultra-violet radiation of 123 nm via a UV resonance lamp. We flow a mixture of 10% Kr and 90% He gas at 0.6 Torr through the

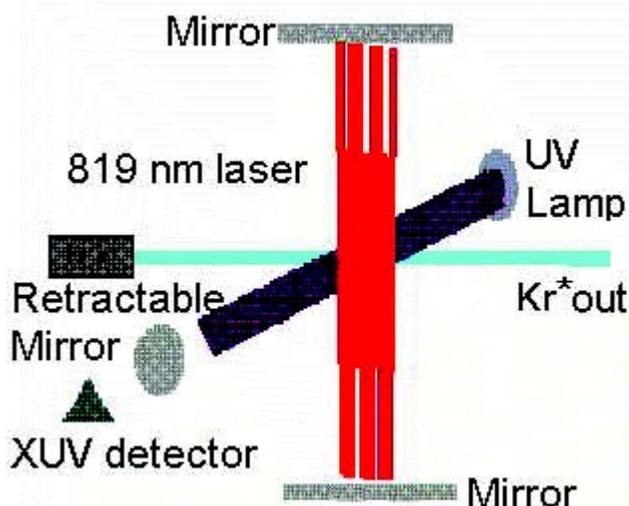


Figure 1: Experimental Setup I: Production of Metastable Krypton Beam

lamp and inject a 65W microwave to excite the gas mixture for ultraviolet emission. The lamp itself has a magnesium fluoride exit window for UV transmittance. The values are, again, from the Young et al. (2002) paper, and adjusted to have maximum value on the XUV detector (seen in figure 1). The 819 nm photons are sent in from a Ti:Sapphire ring laser, operating typically at 300 mW. To reduce noise signals from the various detectors, however, we chop the infrared laser at 1275 Hz, to get an average power of around 150 mW. Using an external lens, we can broaden the laser beam size to 6 mm, comparable to that of the atomic beam size. The beams are sent in normal to the atomic beam path to reduce the effects of Doppler shifting and provide maximal signal at resonance.

The presence of Kr^* is inferred from the 760 nm fluorescence emitted when the krypton atom decays from the 5p J=2 state to the metastable state (see figure 3). Once the

krypton is optically pumped to the 5p J=2 state, there is a 77% branching probability that it will settle into the Kr^* state. Detection of the 760 nm fluorescence is accomplished by a focusing lens at 5 cm from the interaction region that projects the fluorescence onto the photodiode which is fitted with an interference filter that passes about 50% of the 760 nm photons. A measurement at 800 nm showed the photodiode to be sensitive to 0.4 mA of current output per 1 mW of input power, or that each picoampere of current corresponds to about 10^7 incident photons per second.

Once the presence of Kr^* is established, more precise counting can be accomplished through the 811 nm cyclical absorption-emission of the Kr^* as seen in figure 2. In the probe chamber, a 811 nm diode laser crosses the krypton beam. The cyclical transition provides a good indication of the number of Kr^* that arrive in the second chamber.

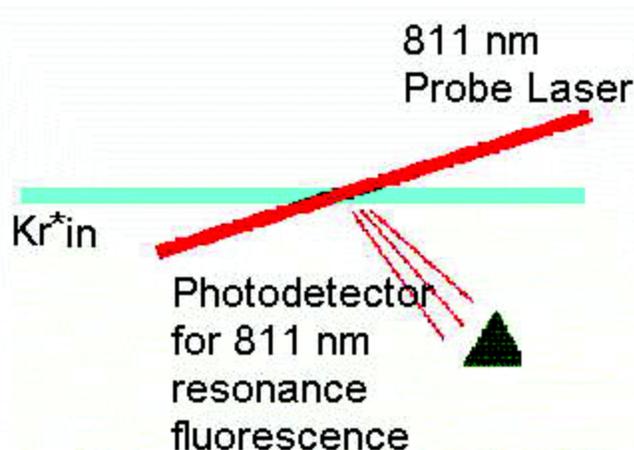


Figure 2: Experimental Setup II: Detection and Counting of Metastable Krypton in the Beam

RESULTS

The results of the experiment seem to confirm the feasibility of metastable rare gas atomic beam production through optical methods, yet much work is still needed to surpass the production rate of current rf-discharge methods. At the sensitivity available, we are able to observe a discernable signal down to pressures of 1.5 mTorr. The signal is established by scanning the Ti:Sapphire laser across a 0.007 nm band centered at the resonance frequency of 819.2303 nm. Because of the velocity distribution of the thermal atoms in the beam, it is expected, and observed, to have a Gaussian profile with respect to frequency. The limit observed at 1.5 mTorr is due to the background noise of the instruments, such as the electrical noise associated with the amplifiers,

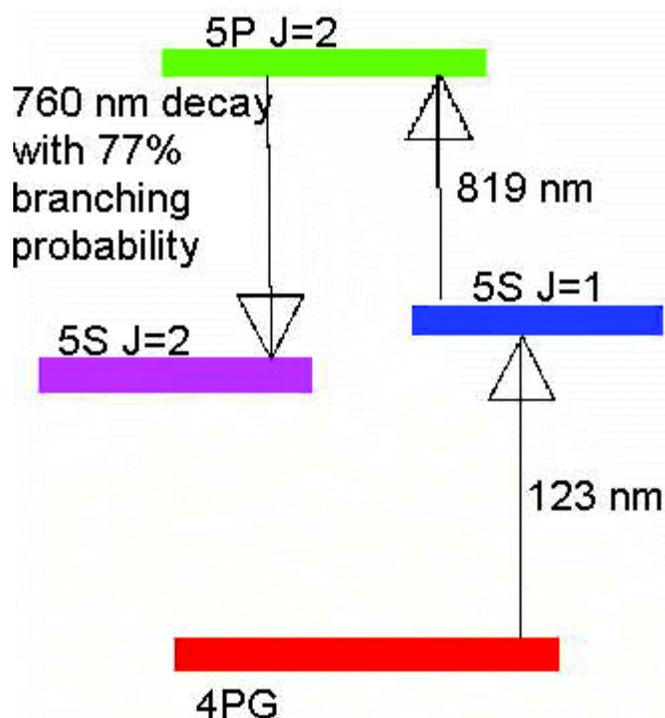


Figure 3: The excitation pathway to arrive at the 5s J=2 state. First excite the ground state with an ultra-violet photon to 5s J=1, and excite that within 4ns to 5p J=2 with an infrared photon. Finally, the atom decays into the metastable state by emitting an infrared fluorescence with 77% branching probability.

and the random photon scatterings originating from the UV lamp. At below 1.5 mTorr, the noise is much larger than the signal, which was ascertained when the sum of repeated data runs approaches a flat line. At the central peak at 1.5 mTorr, we observed a signal size of 1.3 pA. At higher pressures, the increase in signal size is comparable to the UV absorption observed in the Young et al. (2002) paper. For example, at 4.1 mTorr, we observed a signal size of 2 pA, and at 2.3 mTorr, we observed one of 1.4 pA.

Calculations assuming isotropic emission of the 760 nm fluorescence, zero attenuation of the signal from the Kr* gas present, and zero attenuation from the lens material, as well as an idealized lens showed a reasonable figure. The lens is placed 5 cm from the interaction region, and the aperture on the photodiode is 11.6 mm in diameter, which computes to a 4×10^{-2} sr observation window. Factoring in our previously calculated 1pA to 10^7 photons per second conversion, and the 50% attenuation of the pass filter, we arrive at 10^{10} photons per second total as a lower bound. On the other hand, if the lens failed to focus at the infrared wavelength, an upper bound established by that is on the order of 10^{12} photons per second. Running in similar conditions as the rf-discharge (Chen et al., 2001), our preliminary, yet to be optimized production rate (4×10^{10} photons per sec) is already approaching the value of the rf (10^{11}) within an order of magnitude.

At 4 mTorr pressure, the thermal atoms still have Doppler profiles in the direction normal to the beam. Yet in this beam form, we collected data that are similar in form to, albeit smaller in value than the data presented in Young et al. (2002). As mentioned earlier, this apparatus is far from optimized. By extrapolation using the data from Young et al. (2002), it is very possible that we can produce Kr atoms at pressures well below 1.5 mTorr; however, we are currently limited by noise from observing the presence of Kr* atoms at lower pressures. The main source of the noise is from the higher energy transitions of krypton gas in the UV lamp, which produces infrared photons in resonance with those we are trying to observe. Because the UV lamp is not a directed source of light, infrared photons have high probability of surviving multiple reflections inside the stainless steel chambers. This might be overcome in future experiments by painting the inside of the chamber black, or if technology permits, the use of UV lasers.

Because of the 50 cm distance between the two chambers, only at pressures below 0.1 mTorr will the quenching interactions between Kr and Kr* yield a mean free path that allows any significant amount of Kr* to survive into the second chamber. At such pressure, the predicted level of signal falls lower than instrument noise, and is not detectable with our current apparatus, so tests in this regime were inconclusive. As the pressure drops, moreover, the transverse thermal velocity becomes smaller, and so do the wings of the Doppler profile. Currently we have a Gaussian whose width is 700 MHz. In low pressures, the resonant frequency will approach a line frequency, thus enabling a frequency specific scan of fine structure and/or isotopic difference. This can enable us to perform rare isotope trace analysis by loading specific metastable isotopes into a magneto optical trap.

Future optimization for the system will first focus mainly on the noise reduction. Besides painting the interaction chamber black, as mentioned above, there is also the possibility of optimizing the UV lamp. In the experiments documented in the paper, the readings on the UV detector indicated an abnormally small absorption of the UV light by the krypton gas in the chamber, as compared with the data in the Young et al. (2002) paper. Also, the net UV production is smaller than expected (Young et al., 2002). It is possible that with our current configuration, the UV producing region of the lamp is not at its best position possible, (Young et al., 2002) such that a significant portion of the UV radiation is absorbed by a cushion of krypton gas near the window of the lamp. All such optimization must be taken into consideration before a fully efficient source of metastable rare gas atoms can be made available.

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Madhu Dhar has an undergraduate degree in Chemistry (University of Poona, India). She went on to do graduate and postgraduate work in Chemistry (University of Poona, India), with specialization in Molecular Biology and Genetic Engineering. She started her postgraduate work in the Biochemistry Department at the University of Tennessee and later moved to the Graduate School of Genome Science and Technology/Mammalian Genetics at the Oak Ridge National Laboratory. She is currently a Research Assistant Professor and has a grant from the National Institute of Health funding her research on "Novel Mouse Models of Obesity and Diabetes". She has discovered a novel mouse model and a candidate gene responsible for the obesity and diabetic phenotypes observed in specific radiation-induced deletions maintained at the Oak Ridge National Laboratory.

EVALUATION OF THE GENETIC AND NUTRITIONAL CONTROL OF OBESITY AND TYPE 2 DIABETES IN A NOVEL MOUSE MODEL ON CHROMOSOME 7: AN INSIGHT INTO INSULIN SIGNALING AND GLUCOSE HOMEOSTASIS

SARAH NELSON AND MADHU DHAR

ABSTRACT

Obesity is the main cause of type 2 diabetes, accounting for 90-95% of all diabetes cases in the US. Human obesity is a complex trait and can be studied using appropriate mouse models. A novel polygenic mouse model for studying the genetic and environmental contributions to and the physiological ramifications of obesity and related phenotypes is found in specific lines of mice bred and maintained at Oak Ridge National Laboratory. Heterozygous mice with a maternally inherited copy of two radiation-induced deletions in the *p* region of mouse chromosome 7, $p^{23DF10D}$ and p^{30PUb} , have significantly greater body fat and show hyperinsulinemia compared to the wild-type. A single gene, *Atp10c*, maps to this critical region and codes for a putative aminophospholipid translocase. Biochemical and molecular studies were initiated to gain insight into obesity and glucose homeostasis in these animals and to study the biological role of *Atp10c* in creating these phenotypes. Glucose and insulin tolerance tests were standardized for the heterozygous $p^{23DF10D}$ and control mice on a custom-made diet containing 20% protein, 70% carbohydrate, and 10% fat (kcal). *Atp10c* expression profiles were also generated using Reverse-Transcriptase Polymerase Chain Reaction (RT-PCR). Heterozygous $p^{23DF10D}$ animals showed insulin resistance after receiving a dose of either 0.375 or 0.75 U/kg Iletin R insulin. RT-PCR data also shows differences in *Atp10c* expression in the mutants versus control mice. Using these standardized biochemical assays, future studies will further the understanding of genetic and nutritional controls of glucose homeostasis and obesity in animal models and subsequently in human populations.

INTRODUCTION

Obesity is a growing health concern for today's society, due partly to its causal relationship to non-insulin dependent type 2 diabetes and cardiovascular disease. Recently, the U.S. Surgeon General reported that 61% percent of Americans are obese (Berger 2002). In addition, there are over 16 million cases of diabetes in the United States, 90-95% of which are type 2 diabetes (McLaughlin 2001). As with other complex traits, obesity and diabetes in humans are due to

complex interactions between genetic and environmental factors. Despite the polygenic nature of these disorders, genetic assays related to quantitative trait loci (QTL's- specific regions of chromosomes containing a gene or genes that are involved in a complex phenotype without being solely responsible for that phenotype) are helpful in determining their cause, course, and affect (Dhar 2002).

Since 1949, the Mammalian Genetics Section at Oak Ridge National Lab (ORNL) has created and maintained a large number of mouse strains carrying radiation-induced, chromosomal deletions. To date, over 100 mutations have

been isolated in the *p* region of chromosome 7, shown through QTL's to be a critical region for affecting body fat in mice. Dhar et al. have identified and mapped a novel gene to this region, *Atp10c*, that codes for a putative aminophospholipid translocase (ATPase). This protein product is involved in the modulation of body fat through its role in transporting phospholipids across cell membranes (Herzing et al. 2001). Two specific homozygous lethal deletions studied by Dhar et al., $p^{23DFIOD}$ and p^{30PUB} (deletions of the promoter and first two exons and of the entire *Atp10c* gene, respectively- see Figure 1), have been shown to lead to obesity and diabetes-related phenotypes in affected mice. The maternal inheritance of either the $p^{23DFIOD}$ or p^{30PUB} mutation causes heterozygous mice to become visibly fatter as they age and exhibit hyperinsulinemia and hyperglycemia (Dhar 2002). The paternal inheritance of the same deletions renders the pups null for obesity and diabetes-related phenotypes, suggesting paternal imprinting (maternal expression), or "gene silencing."

Unlike other mouse models for obesity, these deletions correspond to a maternally expressed human orthologue on chromosome 15 related to Angelman Syndrome, a neurobehavioral disease (Meguro et al. 2001). A subset of those affected by AS also exhibit obesity, leading researchers to hypothesize that a lack of *ATP10C* expression in brain tissues may be involved in obesity. Dhar et al. have suggested that in both mice and humans, the expression of this novel aminophospholipid translocase plays a role in the metabolism of fatty acids and is therefore relevant to obesity and diabetes.

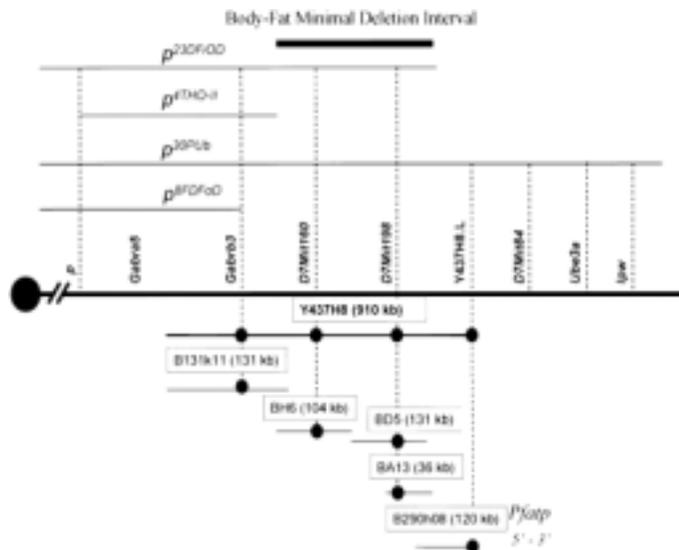


Figure 1. A genetic and physical map of the $p^{23DFIOD}$ and p^{30PUB} deletions in the *p* region of murine chromosome 7. Yeast and bacteria artificial chromosomes (YACs and BACs, respectively) mapped to this area are also shown. Adapted from: Dhar, Madhu, Webb, L., Smith, L., Hauser, L. Johnson, D., West, D.B (2000). A novel ATPase on mouse chromosome 7 is a candidate gene for increased body fat. *Physiological Genomics*, 4, 93-100.

Product Number:	LabDiet 5001*		ResearchDiet D12450B	
Kcal/gm:	3.04		3.85	
Nutritional Info	gm %	kcal %	gm %	kcal %
Protein	23.4	28.049	19.2	20
Carbohydrate	49.9	59.814	67.3	70
Corn Starch	31.9		33.2	34.5
Sucrose	3.68		33.2	34.5
Fat**	4.5	12.137	4.3	10
-lard/animal fat			1.896	4.44
-soybean oil			2.37	5.55
Nitrogen Free Extract	49.9		75.1	
Fiber	5-20		4.7 (cellulose)	0

	Saturated fat	Monosaturated fat	Polyunsaturated fat
Lard (animal)	37%	46%	11%
Soybean (vegetable)	14%	24%	61%

*Lab Diet is a closed formula that can vary from batch to batch. Fiber can range from 5-20% and the fiber is from digestible and non-digestible sources. Protein, fat, carbohydrates, ash, added and mineral can also vary from batch to batch.

** Lab Diet 5001 (regular chow) has animal fat as main fat source. By wt. %age, regular chow is 1.50% saturated fatty acids, 1.58% monounsaturated fatty acids, and 0.26 % Omega-3 fatty acids. Research Diet D12450B gives following breakdown of fatty acids:

Table 1. Nutritional components of regular lab chow vs. custom made diet.

METHODS

Mice containing the radiation-induced, Oak Ridge $p^{23DFIOD}$ deletion (notated pxpl, indicating a maternally inherited deletion unless notated pxpl-pdel, meaning a paternal deletion) were monitored and weighed every two weeks, along with control mice (notated ppx). Thirty-four mice (males: 6 ppx, 8 pxpl, 2 pxpl-pdel; females: 10 ppx, 5 pxpl, 3 pxpl-pdel) were maintained on the regular chow fed to all mice in the facility, LabDiet 5001. Others (males: 8 ppx, 15 pxpl; females: 5 ppx, 5 pxpl), after reaching 5-7 weeks, were placed on custom made, Research Diet D12450B (referred to as the yellow diet) containing slightly less fat and more carbohydrate. (For specific nutritional breakdowns of these two diets, see Table 1). The weight gain of ppx vs. pxpl on both the regular and the special diet was monitored and recorded.

Mice from both experimental and control groups were sacrificed and dissected. Their tissues (heart, liver, kidney, spleen, pancreas, inguinal fat, epididymal fat, cerebellum, hippocampus, and the rest of the brain) were removed and snap frozen with liquid N_2 , collected for RNA expression analysis. Immediately following CO_2 asphyxiation, blood was collected from the heart to be sent for off-site lipid analyses (HDLs, LDLs, etc). The fat depots (see Figure 2) were collected and used to calculate the adiposity index (AI)- a crude measure of body fat. (See Dhar et al. 2000)

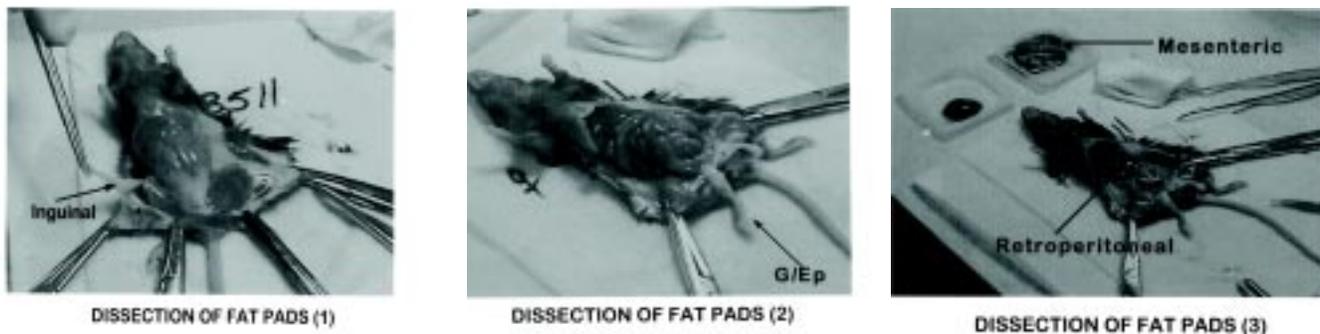


Figure 2. Fat depots collected and weighed during dissection. A) inguinal (subcutaneous) fat. B) epididymal (gonadal) fat. C) mesenteric and retroperitoneal fat depots.

MOLECULAR ANALYSIS

RNA was extracted from mouse tissues and quantitated using the protocol for Preparation of Total RNA Using the GIT CsCl Step-Gradient technique (Bultman 1990).

RT-PCR was used to analyze the level of expression of *Atp10c* in different mouse tissues, using b- actin and *Ube3a* as controls (See Dhar et al. 2000). ORNL primers 827/829 were used for *Atp10C*, 559/560 for b- actin, and 605/606 for *Ube3a*.

BIOCHEMICAL ANALYSIS

Glucose tolerance tests and insulin tolerance tests were used to determine the presence of diabetic phenotypes in the mice. The protocol for glucose tolerance testing was standardized as follows: mice were fasted overnight (at least 16 hours), after which a tail bleed was induced using a surgical blade. Blood glucose was measured (time 0) using the commercially available OneTouch Ultra Brand meter and FastTake test strips. Mice were then subcutaneously injected with a glucose solution (2 g/kg) and blood glucose

readings were taken again at each of the following time points: 30, 60, 90, 120 and/or 150 min (dependent on whether glucose had returned to within the normal range). Data was entered into Microsoft Excel and line graphs were plotted of the average responses. Results were entered into StatView, undergoing the ANOVA Factorial test to determine statistical significance between ppxx and pxpl responses at each time point.

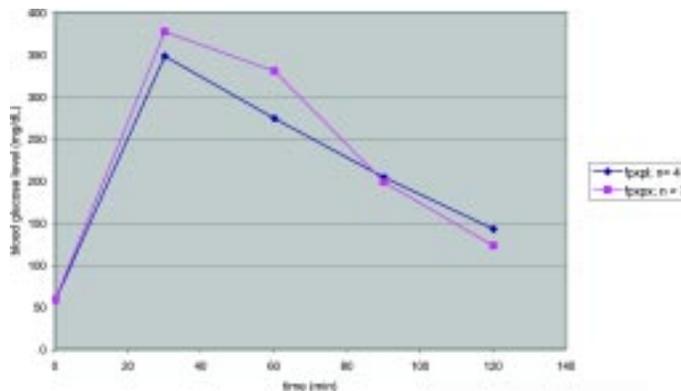


Figure 4. Glucose Tolerance Test (2 g/kg) in overnight fasted, 4-6 mo. 23D females on regular chow, ppxx vs. pxpl.

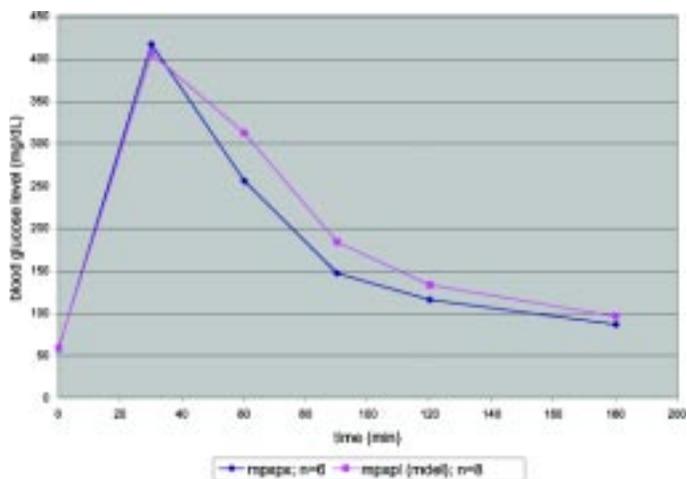


Figure 3. Glucose Tolerance (2 g/kg) Test in overnight fasted 10-12 mo. Old 23 D males on regular chow, ppxx vs. pxpl.

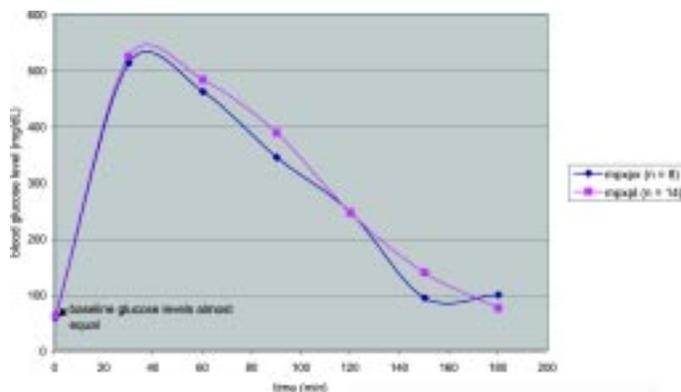


Figure 5. Glucose Tolerance Test (2 g/kg) in overnight fasted, 4-6 mo. 23D males on yellow diet, ppxx vs. pxpl.

RESULTS

This research initiated and standardized biochemical analyses for the study of insulin signaling and glucose homeostasis in $p^{23DFioD}$ mice on a custom-made diet. Figure 3 shows results of the glucose tolerance test (2 g/kg) in 10-12 month ppx and pxpl males on LabDiet 5001; results for 4-6 month females on the same diet is shown in Figure 4. Figure 5 shows the glucose tolerance test in 4-6 month males on ResearchDiet D12450B, and Figure 6 shows results for the same test in 4-6 month females. No statistical significance exists between ppx and pxpl averages at any time point in the glucose tolerance tests for males or females on either diet.

Insulin tolerance test results (0.75 U/kg, fasted 2 hours) for 10-12 month males on LabDiet 5001 are shown in Figure 7. The average blood glucose level in the mutants is significantly higher at 120 minutes ($p < 0.5$). Figure 8 shows the same test in 4-6 month old males on the custom-made diet,

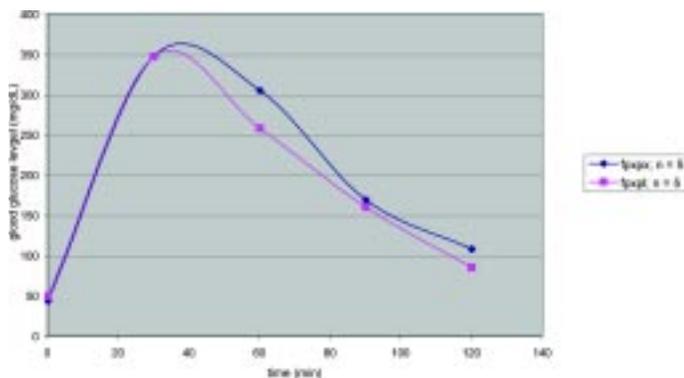


Figure 6. Glucose Tolerance Test (2 g/kg) in overnight-fasted, 4-6 mo. 23D females on yellow diet, ppx vs. pxpl.

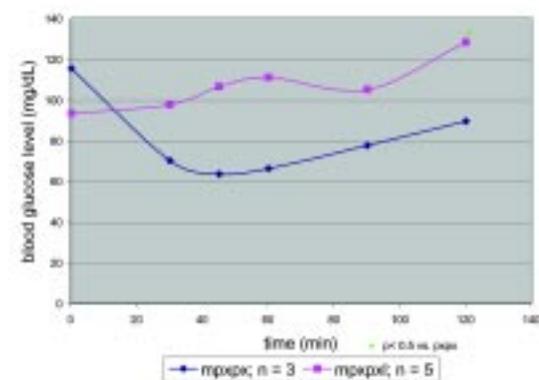


Figure 7. Insulin Tolerance Test (.075U/kg) in 2 hour fasted, 10-12 mo. 23D males on regular chow, ppx vs. pxpl.

with no statistical significance at any time point. Insulin tolerance test results for 4-6 month females on the custom-made diet is shown in Figure 9. At 90 minutes, 3 out of 4 ppx animals went into insulin shock and had to be injected subcutaneously with a glucose solution. For these animals, blood glucose level was not measured at 120 minutes. A lower dosage of insulin (0.375 U/kg) was used for the insulin tolerance test in 4-6 month males on the custom diet, shown in Figure 10. Here, the pxpl animals were significantly higher ($p = 0.0362$) at 120 minutes.

The RT-PCR expression profile for *Atp10c*, as compared to b-actin *Ube3a*, in a ppx and pxpl mouse is shown in Figure 11.

CONCLUSIONS

TESTS WERE INITIATED AND STANDARDIZED

Mice carrying a maternally inherited copy of the $p^{23DFioD}$ deletion have been shown to have significantly greater body fat than either the wild type or mice with a paternally inherited copy of the deletion. These studies were the first step towards looking at the effects of nutritional variables in the physiology of these mice. The experiments standardized in this work will further the investigation of a possible obesity-related, type 2 diabetic phenotype in this mouse model already recognized for polygenic obesity. Insulin and glucose tolerance tests were standardized for animals on the custom made diet because laboratory chow is not consistent enough from batch to batch to use in a study of nutritional variables. ResearchDiet D12450B contains a fixed amount of fat, carbohydrate, and protein, making it a better diet to use for nutritional comparisons.

Glucose tolerance tests appear normal while insulin tolerance tests suggest a trend of insulin resistance in $p^{23DFioD}$ mice.

In the glucose tolerance test, mutant and control mice were virtually indistinguishable in their responses, indicating that there is no apparent defect in glucose metabolism in these mice. The insulin tolerance tests, however, suggest that there may be some defect in the insulin response pathway related to the $p^{23DFioD}$ deletion. Males 10-12 months old on the regular chow show statistical significance ($p = .04$) as compared to the ppx animals at 120 minutes in the insulin tolerance test. Their increased blood glucose levels at these latter time points could suggest insulin resistance- a phenotype associated with type 2 diabetes. Younger males on the custom-made diet showed significance at 120 minutes when tested with a lower dosage of insulin (0.375 U/kg), but did not exhibit the phenotype on the higher dosage (0.75 U/kg). This phenomenon may be understood by considering the use of insulin injections as a treatment for insulin resistance in type 2 diabetics. A decreased efficiency in insulin response is treated by essentially overwhelming the system

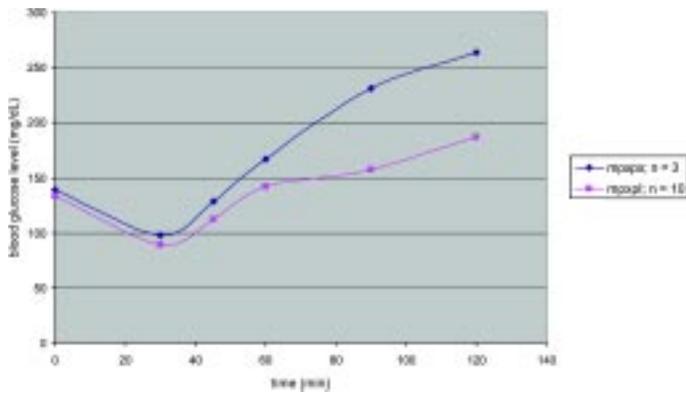


Figure 8. Insulin Tolerance Test (0.75U/kg) in 2 hour fasted, 4-6 mo. 23D males on yellow diet, ppxx vs. pxpl.

with insulin, maximizing the insulin induced transport of glucose from the bloodstream into the body cells by “occupying” every available insulin receptor with a steady supply of insulin. At the higher dosage, the younger mice may have been receiving a high enough concentration of insulin to mask any insulin resistance. In humans with type 2 diabetes, it is known that insulin resistance often increases with age—rendering lower dosages of insulin less effective in older patients. It may be for this reason that the 10-12 month males showed a trend of insulin resistance at the higher dosage.

Figure 7 illustrates the trend of insulin resistance seen in the 10-12 month old mice. Thirty minutes after the insulin injection, the blood sugar of the control mice dropped to an average of 65 mg/dL, while the mutants were maintaining levels near 100 mg/dL. A particularly interesting trend was found in females on the custom diet, shown in Figure 9. Three out of 4 controls were in danger of hypoglycemic shock 90 minutes after the insulin injection (0.75 U/kg) and had to be given glucose. All 4 mutants were still visibly active at this time, and while their blood sugar level was still lower than normal fasting level, they showed a significantly

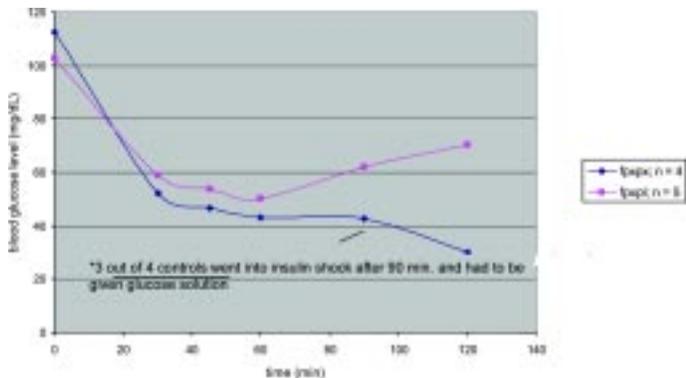


Figure 9. Insulin Tolerance Test (0.75U/kg) in 2 hour fasted, 4-6 mo. 23D females on yellow diet, ppxx vs. pxpl.

diminished response to the insulin. Although not statistically significant, the results from these females suggest also suggest a trend of insulin resistance. This data is preliminary; however, and more animals need to be added to these studies before conclusions can be made in regard to the role of the $p^{23DFloD}$ deletion in the glucose-insulin pathway.

Little is known about the biological role of translocases, such as the one coded for by *Atp10c*, other than that they somehow alter the orientation of receptor molecules in the cell membrane. Based on the knowledge of the cellular signaling involved in the insulin pathway, lipolysis, and general lipid metabolism, it seems reasonable to suggest that this class V putative aminophospholipid translocase may be involved in creating a diabetes-related insulin resistance, in addition to obesity. Kahn et al. (2000) suggest that even though insulin resistance is characteristic of obesity and type 2 diabetes, it may not be that all of insulin’s actions are

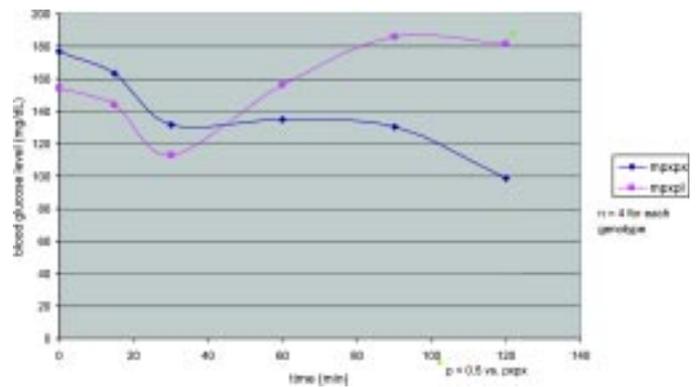


Figure 10. Insulin Tolerance Test (0.037U/kg) in 2 hours fasted, 4-6 mo. 23D males on yellow diet, ppxx vs. pxpl.

affected in people with these conditions. The varied roles of insulin in the body may explain why these mice show impaired insulin response in insulin tolerance tests while exhibiting a normal profile in the glucose tolerance tests. Glucose homeostasis involves complex pathways, and although these mice do not exhibit all the symptoms associated with type 2 diabetes, their abnormal responses in the insulin tolerance test may elucidate the role of *Atp10c* in physiological responses characteristic of obesity-related diabetes.

MUTANT SHOWS DECREASED *ATP10C* EXPRESSION.

The RT-PCR results of the pxpl animal on the custom diet show decreased expression of *Atp10c* in liver, cerebellum, and inguinal and epididymal fat depots. Based on this pxpl animal, the observation can be made that a decreased amount of *Atp10c* in the fat depots is associated with increased body fat (larger fat depots). The inverse relationship seen between expression in the fat tissue and the size of the

fat depots seems logical in light of *Atp10c*'s role in lipid metabolism.

These results, however, compare only one ppx animal to one pxpl. These results need to be repeated before any conclusions are drawn. For example, the ppx shows decreased expression in the pancreas as compared to the pxpl. It is debatable whether this decreased band intensity is truly due to lower expression or rather to degradation of the sample.

FUTURE DIRECTIONS

Now that the actions of glucose and insulin in relation to *Atp10c* for $p^{23DFioD}$ mice on a custom made diet have been studied, experiments are underway to observe the effects of nutritional variables. Several $p^{23DFioD}$ mice have been placed on a high fat (45% kcal) diet. Glucose and insulin tolerance tests are in progress for these animals, whose results will be

compared to mice on ResearchDiet D12450B (10% kcal). High fat diets have been shown to increase adiposity and are known to aggravate symptoms of type 2 diabetes in humans. Preliminary tests in $p^{23DFioD}$ mice on the high fat diet for 4 weeks already show significant insulin resistance (from 30 minutes onward) and an abnormal profile in the glucose tolerance test. The hypothesis for these experiments is that the high fat diet will induce more severe diabetes-related phenotypes and increased fat depots in $p^{23DFioD}$ mice.

Until recently it has been difficult to generate many pups containing the longer deletion, p^{30PUB} - shown to cause a more severe form of obesity than that seen in the $p^{23DFioD}$ animals. These pups are now being bred more successfully and included in the high-fat diet study. Preliminary data from 2 p^{30PUB} animals (as compared to $p^{23DFioD}$ controls) show an abnormal glucose tolerance test, suggesting trends of hyperglycemia ($p = 0.0014$ at 0 min.) and glucose intolerance ($p < 0.5$ at 30 and 60 min.) in these mice. This is in addition to the insulin resistance and hyperinsulinemia also seen in the shorter deletion. Preliminary insulin tolerance tests in the p^{30PUB} animals show significant insulin resistance from 60 minutes onward ($p = 0.00200$ at 60 min., 0.0243 at 90 min., and 0.0021 at 120 min.). With the presence of p^{30PUB} controls and more animals carrying the deletion, future glucose and insulin tolerance tests results may show that these animals provide a better mouse model for obesity-induced type 2 diabetes in humans.

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My gratitude also goes to the US Department of Energy and the National Science Foundation for funding the Energy Research Undergraduate Laboratory Fellowship (ERULF)- a program in which I have been honored to take part. I would also like to thank the staff of Oak Ridge Institute for Science and Education (ORISE)- especially Linda Holmes and Cheryl Terry- for all the work they have put into this summer's program.

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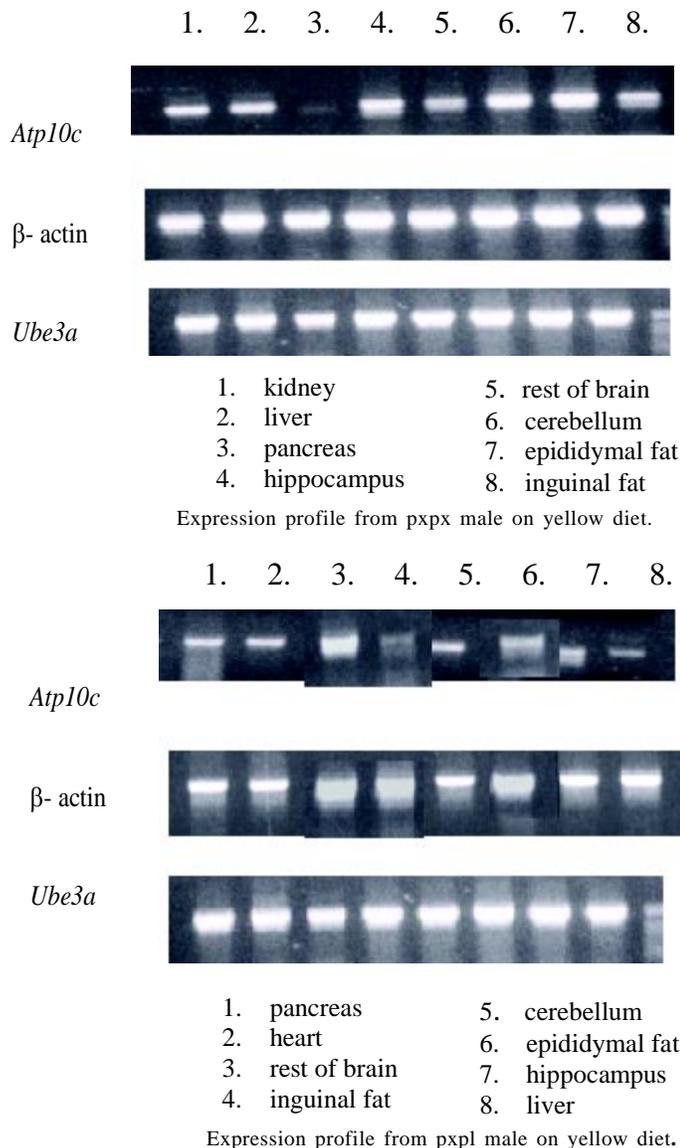


Figure 11. RT-PCR *Atp10c* expression profiles for ppx and pxpl mice on yellow Research Diet.

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Anh Quach has an undergraduate degree in Chemical Engineering from the University of Arizona, 2003. While attending University of Arizona, she was involved in various research projects, including surface modifications to be used in separation techniques, as well as the encapsulation of waste in a polymer matrix. The latter project derived from her participation in the NSF/DOE Faculty and Student Team Program at Pacific Northwest National Laboratory. The research conducted resulted in a poster presentation at the AAAS National Conference in 2003, and two oral presentations at the American Society of Ceramics Engineers National Meeting, 2003.

Dunbar Birnie has both undergraduate and graduate degrees from MIT in Materials Science and Engineering. After receiving his Ph.D. in 1986 he joined the faculty at The University of Arizona. He has extensive experience in making and examining thin films, with major emphasis on sol-gel derived coatings of many different compositions. Throughout his career, he has been active at promoting undergraduate student involvement in hands-on research experiences. He often has undergraduates working with him on laboratory projects and many of these projects ultimately lead to publication or presentation at national meetings.

Wendell Ela received his B.Sc. degree in Civil and Environmental Engineering from Virginia Polytechnic Institute. He completed both his Masters and Ph.D. degrees from Stanford University in Environmental Engineering where his thesis focused on how particles interact in aqueous environments. Now an Assistant Professor at The University of Arizona in the Chemical and Environmental Engineering Department, he specializes in water and wastewater treatment processes with a particular interest in developing field applications for innovative laboratory technologies. Some of his and his students' current projects involve application of electrochemical and photochemical techniques to groundwater cleanup, laboratory simulation of toxics leaching from landfills, development of stabilization methods for toxics disposal, and fabrication of automated infiltrometers for reclaimed water recharge basins.

Eduardo Sáez has a Ph.D. in Chemical Engineering from the University of California at Davis, 1984. He has been a faculty member in Chemical Engineering at Universidad Simón Bolívar in Caracas, Venezuela, North Carolina State University and is currently Associate Professor at the University of Arizona. In 1992 he held a Marie Curie Scholar position in the Department of Physics at the University of Bristol. His current research involves transport in colloidal and multiphase systems and rheology of polymer and surfactant solutions.

Brian J.J. Zelinski earned his Ph.D. in Ceramic Science at the Massachusetts Institute of Technology in 1987. He is currently an associate professor in the Materials Science and Engineering Department at the University of Arizona. His research interests include the wet chemical synthesis and characterization of piezoelectric, ferroelectric, electronic, and optical thin films, the kinetics of phase transformations, interfacial interactions between metal/ceramic/organic interfaces, and the sol-gel synthesis of organic and inorganic materials. In collaborative work with PNNL, he has developed techniques for fabricating hybrid polyceramic materials for potential application in nuclear waste storage and site remediation and decommissioning.

DEVELOPMENT OF POLYMERIC WASTE FORMS FOR THE ENCAPSULATION OF TOXIC WASTES USING AN EMULSION-ENCAPSULATION BASED PROCESS

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WENDELL P. ELA, BRIAN J. J. ZELINISKI AND, GORDON XIA, AND HARRY SMITH

ABSTRACT

Developed technologies in vitrification, cement, and polymeric materials manufactured using flammable organic solvents have been used to encapsulate solid wastes, including low-level radioactive materials, but are impractical for high salt-content waste streams (Maio, 1998). In this work, we investigate an emulsification process for producing an aqueous-based polymeric waste form as a preliminary step towards fabricating hybrid organic/inorganic polyceramic matrices. The material developed incorporates epoxy resin and polystyrene-butadiene (PSB) latex to produce a waste form that is non-flammable, light weight, of relatively low cost, and that can be loaded to a relatively high weight content of waste materials. Sodium nitrate was used as a model for the salt waste. Small-scale samples were manufactured and analyzed using leach tests designed to measure the diffusion coefficient and leachability index for the fastest diffusing species in the waste form, the salt ions. The microstructure and composition of the samples were probed using SEM/EDS techniques. The results show that some portion of the salt migrates towards the exterior surfaces of the waste forms during the curing process. A portion of the salt in the interior of the sample is contained in polymer corpuscles or sacs. These sacs are embedded in a polymer matrix phase that contains fine, well-dispersed salt crystals. The diffusion behavior observed in sections of the waste forms indicates that samples prepared using this emulsion process meet or exceed the leachability criteria suggested for low level radioactivity waste forms.

INTRODUCTION

Many industrial processes create wastes containing high concentrations of salts mixed with toxic metals such as cadmium, lead, and arsenic. These processes include semiconductor manufacturing, mining/mineral processing, agricultural desalination, glass manufacturing, and pulp and paper mills, among others. Water treatment utilities use ion removal processes such as packed-bed adsorption, membrane filtration and ion exchange to trap toxic metals and other contaminants in iron or aluminum hydroxide containing sludges or residuals that often contain large quantities of salt. Another source of salt waste includes the 200 million kilograms of chloride, sulfate, and nitrate salts, contaminated with toxic metals and low-level radioactive elements, which are distributed among the various Department of Energy sites around the nation (Maio et. al., 1998). Attempts to dispose

of this low-level radioactive waste generate an additional 5 million kilograms of salt wastes per year.

Disposal of high salt containing waste is problematic because the salt component is vulnerable to leaching and high loadings tend to destabilize most matrices currently used for waste encapsulation. Encapsulation is necessary because the contaminating toxic metals must be prevented from entering the environment in an uncontrolled manner in the unlikely event that the storage facility be compromised. Currently, various types of technologies exist to encapsulate waste. Vitrification requires firing the waste at high temperatures where some toxic components may volatilize. Encapsulation using polymer matrices or composite polymers usually relies on the use of volatile and flammable organic solvents (Conner, 1990). Salt loading in grout is limited because large amounts decrease durability and lead to poor leaching control (Krishnamoorthy et al., 1993, Maio et. al., 1998, Leist et al., 2000).

Organic-inorganic hybrid materials known as polyceramics (i.e., materials that are a mixture of polymer and ceramic components) possess good mechanical integrity, high chemical durability, low processing temperatures (below 100°C), and ease of fabrication, properties which qualify them as candidate materials for encapsulating and storing a wide range of salt wastes. Polyceramics using rubber (butadiene) as the organic component and silica as the ceramic component were first developed as waste forms for salt encapsulation through a joint collaboration between the Arizona Materials Laboratory of the University of Arizona and Pacific Northwest National Laboratory (Smith, Gary L, 1999). These materials greatly exceed the strength requirements specified by the Nuclear Regulatory Commission (NRC) Technical Position Paper for stabilized low-level radioactive waste forms (USNRC 1991). That paper also specifies that the leachability index (a measure of the difficulty of leaching toxic components out

Sample ID	Waste Loading	Water Content
	(wt% NaNO ₃)	(wt. ratio of Water/Polymer)
8L	8	0.5
15L	15	0.5
20L	20	0.5
21H	21	1.5
27H	27	1.5
40I	40	0.75

Table 1. Designation and composition of samples from this study. In the designation, the number refers to the wt% of salt loading in the cured sample and the letter refers to the amount of water in the uncured sample, L: Low, I: Intermediate, H: High.

of the waste form) exceed a value of six. However, a major obstacle to their widespread implementation is the use of highly volatile and flammable organic precursors and solvents in the process flowsheet. To circumvent this problem, work was begun to replace the hazardous organic precursors and solvents with water-borne equivalents to develop environmentally-benign aqueous based processing routes for fabricating durable waste forms (Liang et al., 2002). To date, efforts have focused on fabricating polymer waste forms by cross-linking aqueous emulsions of epoxy and polystyrene-butadiene precursors in the presence of salt waste.

The objectives of this project were to characterize the microstructure of these water-based, epoxy/polystyrene-butadiene polymer waste forms with the intent of identifying how salt is incorporated into their structure and to quantify the rate of leaching of the salt from the waste forms. Most regulatory restrictions address the leaching of toxic metals and other contaminants. However, the salt is likely to be the most mobile species in these waste forms. Thus, quantification of its behavior will represent an upper limit on the amount of leaching to be expected from other slower, less mobile waste form contaminants.

METHODS

To fabricate the samples, polystyrene-butadiene (PSB) latex (BASF, Styronal ND 656), epoxy resin (Buehler, Epo-Kwick Resin), and the surfactant sorbitan monooleate (Span-80) were mixed for 30 minutes to create an emulsion. To this, the cross-linking agent diethylenetriamine (DETA, 99%, Aldrich) and sodium nitrate salt (NaNO_3) were added. This mixture was stirred to uniformity, cast into glass containers and placed in an oven to dry and cure at 80°C until weight loss ceased (typically 3 days). Cured samples were cylindrical and typically weighed 15 g, had diameters of about 2 cm, and lengths of about 3.5 cm. All samples were prepared using equal parts, by weight, of the PSB latex and epoxy resin. A variety of waste forms were prepared having nominal salt loadings in the range of 8-40 wt% of NaNO_3 in the cured samples. The amount of water in the uncured waste forms was also varied in the range of 0.5 to 1.5 wt ratio of water to polymer component (epoxy plus PSB). Table 1 lists the samples and their compositions.

Sample microstructures were characterized using carbon-coated sections using a JEOL 5900 LV SEM with a built-in Everhardt-Thronley (ET) secondary electron (SE) detector and a Robinson series VI scintillation-based backscattered electron (BSE) detector. Compositional data was obtained using an EDAX EDS detector with Genesis v1.0 software with integrated digital imaging and mapping capabilities.

To characterize the leaching behavior of the waste forms, thin sections were extracted from the middle of samples and immersed in a known volume of well-stirred water at 20°C to leach out the salt. The thickness of the thin sections was kept intentionally thin (2.25 to 5.30 mm) to minimize the

time required to characterize the behavior of species having low diffusivities. Measured variation in the conductivity of the liquid was used to determine the amount of salt leached into the solution as a function of time. To determine the total initial salt content samples were leached until variations in the conductivity of the leachate were no longer detected.

The leaching data from the conductivity measurements is interpreted by assuming that the sample is an infinitely long and wide slab with a thickness of $2L$. It is assumed that the sample contains a crust on the exterior of the thin section that dissolves very rapidly in the first moments of leaching. Because the solution is well-stirred, there is a negligible boundary layer in the solution near the surface of the sample, therefore the mass transfer from the sample surface to the liquid is instantaneous, and the salt concentration of the liquid is so small in comparison to that in the sample that it is assumed to be zero. The concentration – time data from the conductivity measurements is interpreted using the infinite slab solution to Fick's 2nd law, adapted to give the fraction of salt still present in the sample after the leaching time t :

(1)

where \bar{c} is the average salt concentration in the sample, c_0 is the initial concentration in the sample, D is the diffusion coefficient, and t is leaching time. The percent of salt retained in the sample, S , does not include the initial fraction of salt in the crust, characterized by the percent P_c :

$$S = \frac{\bar{c}}{c_0} (100 - P_c) \quad (2)$$

The diffusivity and P_c can be fit to experimentally-determined curves of S vs. t . The diffusivity is then used to calculate the leachability index, L_i , defined as:

$$L_i = \log \left(\frac{\beta}{D} \right) \quad (3)$$

where Equation (3) is an appropriate expression for the leachability index as defined by the American National Standards Institute (ANSI/ANS-16.1-1986) assuming that the diffusion coefficient is independent of time during the course of leaching.

RESULTS

Each of the samples listed in Table 1 appear to be homogeneous on a macroscopic scale when visually inspected. Despite this visual homogeneity, SEM analysis revealed that these samples are inhomogeneous at the microscopic scale. Additionally, each sample contains a crust of salt on the external surfaces of the monolith. The characteristics of this crustal layer are shown in Figure 1. In backscattered SEM micrographs, elements with a high atomic number give a stronger signal than elements with low atomic numbers because they contain more electrons. Thus the higher atomic numbered elements show up brighter, or whiter. In this study, the dark regions are polymer and the light regions are salt. As seen in Figure 1, the surface crust may contain a combi-

nation of dendritic crystals which have grown on the exterior of the monolith, large salt crystals in voids or bubbles just below the surface, a continuous layer or coating of salt on the exterior surface, and/or large salt regions just below the surface of the monolith.

To characterize further the microscopic homogeneity of the waste forms, the quantity of salt in various portions of a monolith of sample 40I was determined by sectioning and leaching. Prior to sectioning, the surface salt that was not incorporated into the sample was removed. Table 2 shows the average composition in wt% NaNO_3 for the different sections identified in Figure 2. The top, crustal section of the sample contains the highest concentration of salt at 31.3 wt%. The disk taken from the top but below the crustal disk contains 23.6 wt% salt. Two samples were taken from the middle of the monolith: one was a disk containing the peri-

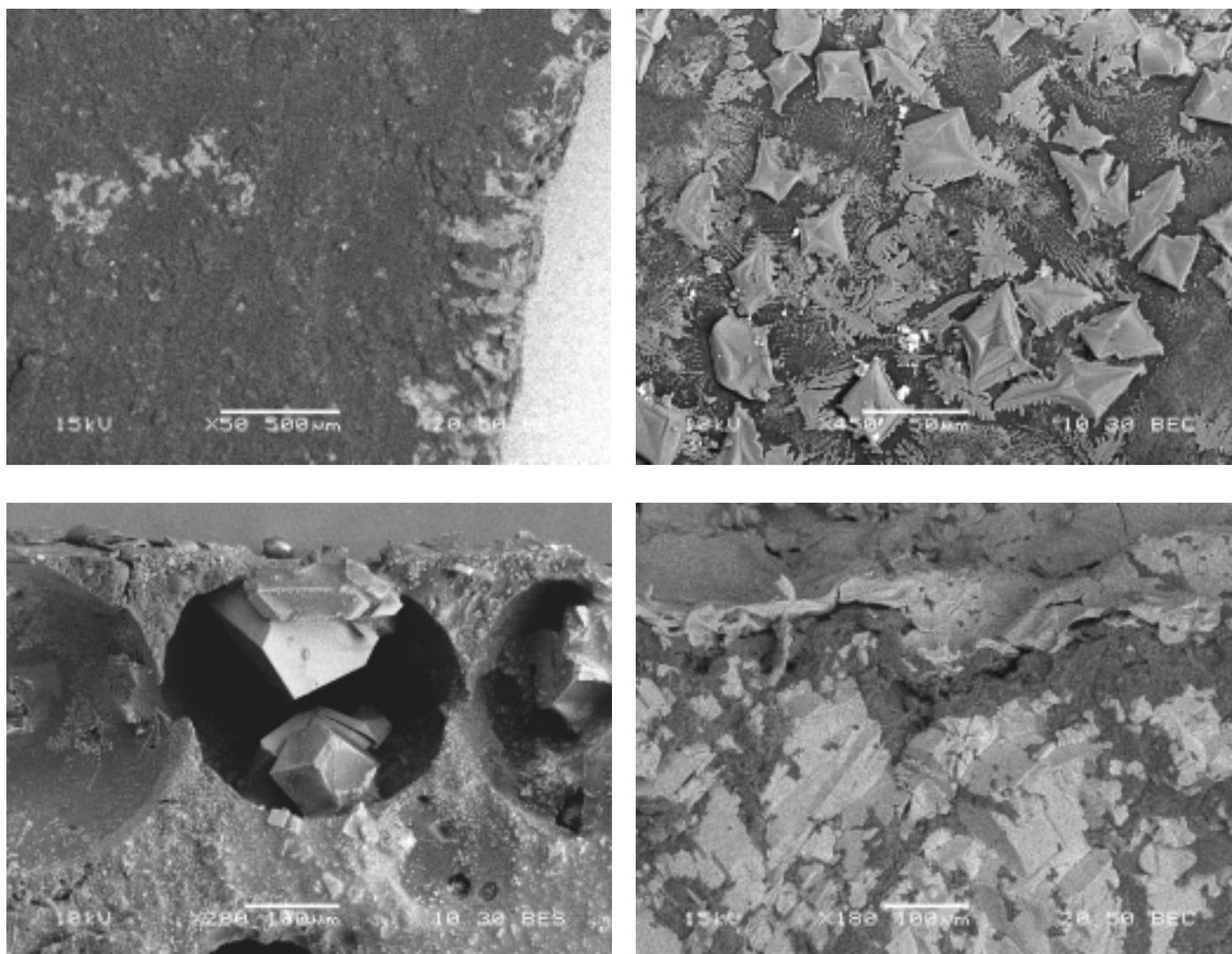


Figure 1. Backscattered SEM images of typical surface crust features: a) cross section containing the external surface of a monolith (vertically oriented at the right) shows a crustal region several hundreds of microns in thickness; b) dendritic crystals growing on external surface; c) large, well-formed salt crystals in near-surface voids; d) continuous layer of salt on external surface with large salt regions just below surface.

meter of the monolith (Section 3), while the other was just the core of the monolith (Section 4). The middle disk has a composition of 17.2 wt% salt while the core contains 9.4 wt% salt. These results confirm that the salt distribution in these waste forms is inhomogeneous, with higher salt concentrations near the external surfaces and lower concentrations in the middle of the waste form.

As seen in Figure 3, the microstructure of the interior or central portion of sample 15L consists of corpuscles or sacs of polymer that are mostly filled with salt. These sacs are embedded in a continuous matrix phase. EDS analysis over large areas (> 100 mm × 100 mm) reveals that the interior of this sample contains about 9.2 wt% salt. A similar result is obtained when the size of the scanned area is reduced so as to sample only the matrix phase between polymer sacs, indicating that the matrix phase contains small, finely dispersed salt crystals. Figure 4 shows the corpuscles or sacs observed in sample 8L. Here the salt crystals inside the sacs are relatively large and possess a well-defined morphology. The interior characteristics of other samples of this study contained similar features, namely corpuscles or sacs of salt embedded in a polymer matrix containing small, well-dispersed salt crystals.

Samples 20L and 27H were prepared in an attempt to increase the salt content in the interior of the waste form. Sample 20L contains sacs of salt similar to those observed in previous samples. However, it also contains a family of pores with sizes in excess of 100 mm (Figure 5). EDS analysis of the interior portions of this sample show that increasing the nominal loading of this waste form does not lead to a corresponding increase in salt content in the interior of the sample. The average composition in the interior of sample 20L was 9.2 wt% salt. Even increasing the target salt loading to 27 wt% did not significantly increase the concentration of salt measured in the center of the waste form monolith. EDS measurements at the center of sample 27H show a composition of 9.8 wt% NaNO₃. Notice that these values agree well with the value of 9.4 wt% measured in the interior or core region of sample 40I as determined by leaching (see Table 2).

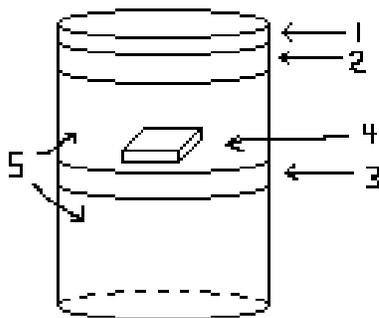


Figure 2. Schematic showing the sections of sample 40I leached to determine average salt content.

Section	Description	% Salt
1	Crust	31.3
2	Top disk	23.6
3	Middle disk	17.2
4	Middle core	9.4
5	Rest of monolith	18.8

Table 2. Salt content (wt% NaNO₃) of various sections of Sample 40I as identified in Figure 2.

The microstructural characteristics of fully leached samples are shown in Figure 6. In both samples 15L and 27H, the polymer corpuscles or sacs appear to be devoid of salt after leaching. EDS analysis indicates that almost all of the salt leaches out of the thin sections used for the leach tests. This indicates that the fine salt crystals distributed in the matrix phase surrounding the sacs leach out as well. After leaching, sample 15L contains approximately 1.3 wt% NaNO₃ and sample 27H contains about 0.7 wt%. Consequently, it seems that at long times, almost all of the salt leaches from these thin sections of the waste forms. Table 3 summarizes the composition analysis obtained by EDS for the interior portions of both the leached and unleached samples of this study.

Figure 7 shows the leaching data, plotted as S vs. t. The model fit is obtained by substituting equation (1) into equation (2), and then fitting D and P_c. Note that the experimental data starts at S=100% at t=0, whereas the model starts at S=100-P_c (i.e., the crustal salt is assumed to be removed instantaneously for modeling purposes).

Table 4 contains the leaching results for samples 15L, 21H and 27H. As seen in the table, the crustal salt of

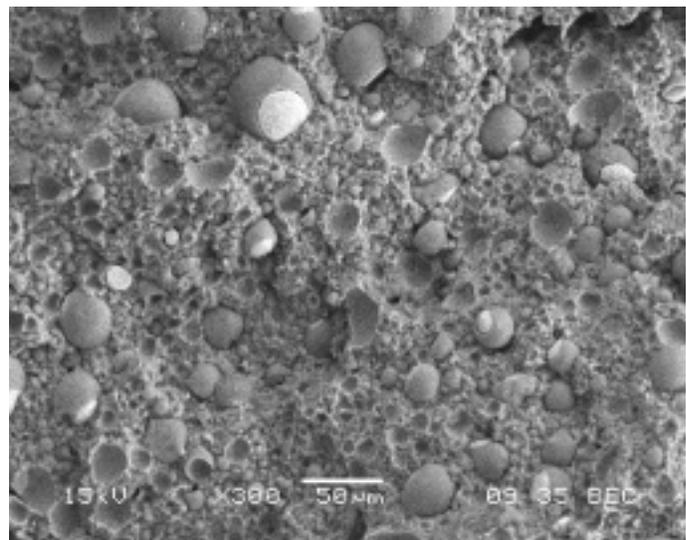


Figure 3. SEM backscattered image of the interior of sample 15L showing corpuscles or sacs of polymer containing salt imbedded in a continuous matrix.

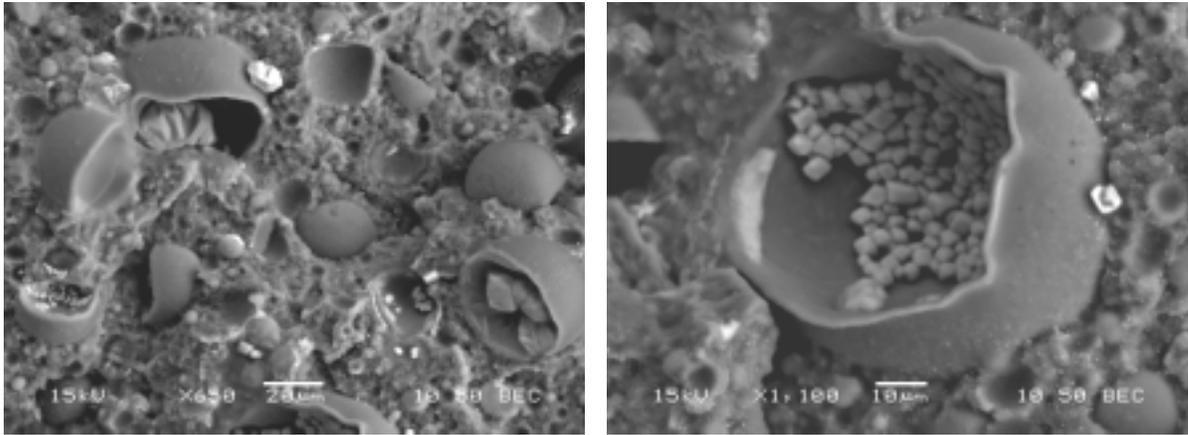


Figure 4. SEM backscattered images of the interior of sample 8L. Compared to 15L, the polymer sacs contain fewer, larger, and better defined salt crystals.

sample 15L made up 1.1% of the original weight of the sample. This quantity of salt leached out of the thin section very quickly and was calculated from the diffusion curve by extrapolation of the long time leach behavior to zero time. The quantity of salt leached from the interior of the sample in a manner consistent with the infinite slab model was calculated to be 9.9 % of the pre-leached sample weight. Taken together, 11 wt% of the sample was extracted during the leaching test. Modeling of the leaching data showed that the interior salt leached from the thin section of sample 15L with a diffusion coefficient of $2.5 \times 10^{-8} \text{ cm}^2/\text{s}$ to give a leachability index of 7.6 as per Equation (3). Analysis of the leaching data for samples 21H and 27H show that slightly more salt was extracted from the crust and interior regions of the sample during leaching than in sample 15L. Although the nominal salt loadings were increased, the amount extracted from the interior of the sample remains at approximately 10 – 12 wt%, a result consistent with EDS measurements of the salt composition at the very core of samples prior to leaching. Comparison of results from the three samples shows that the

diffusion coefficient increases and the leachability index decreases as the nominal salt loading in the waste form increases. However, the leachability index for all samples measured in this study exceeded the value of 6, the minimum value for acceptance as a low level waste form.

CONCLUSIONS

The key to making this material a viable waste form is believed to be the occurrence of a phase inversion during the curing process. Substantial evaporation must occur prior to curing so that the water phase becomes discontinuous and the polymer phase becomes continuous, thus encapsulating the water-soluble salt in the polymeric matrix. Since the water evaporates from the exterior surfaces of the waste form, it migrates from the interior and carries the highly soluble sodium nitrate with it. This migration produces the heterogeneous distribution of salt in the waste form as detected by EDS and measured in the different sections of sample 40I (see Table 2). Evaporation of the concentrated salt solution that migrates towards the surfaces of the waste form causes the formation of the dendritic crystals, cubic crystals, and large regions of embedded salt on or near the surfaces of the waste form as shown in Figure 1.

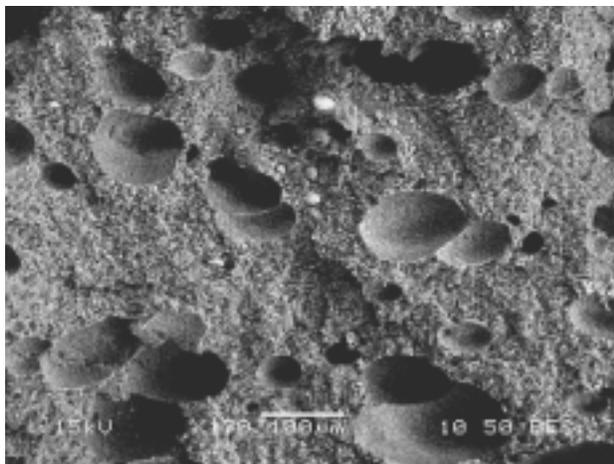


Figure 5. SEM backscattered image of the interior of sample 20L showing large pores.

	Composition (wt% NaNO ₃)	
Sample	Unleached	Leached
15L	9.2	1.3
20L	9.2	-
27H	9.8	0.7

Table 3. Composition of the interior portions of leached and unleached samples as determined by EDS.

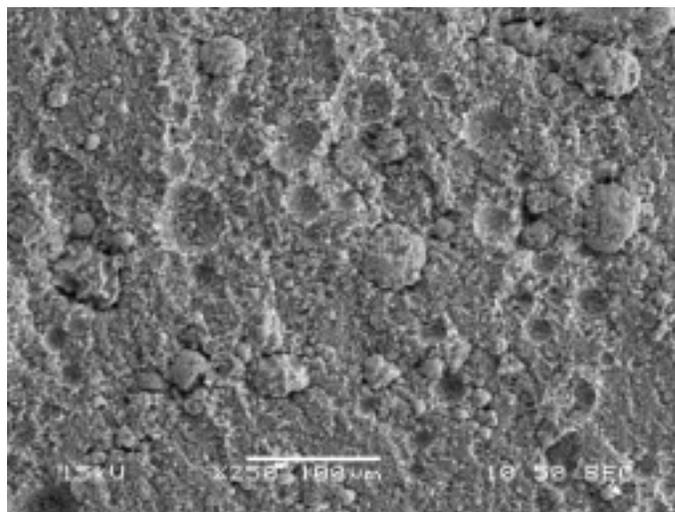
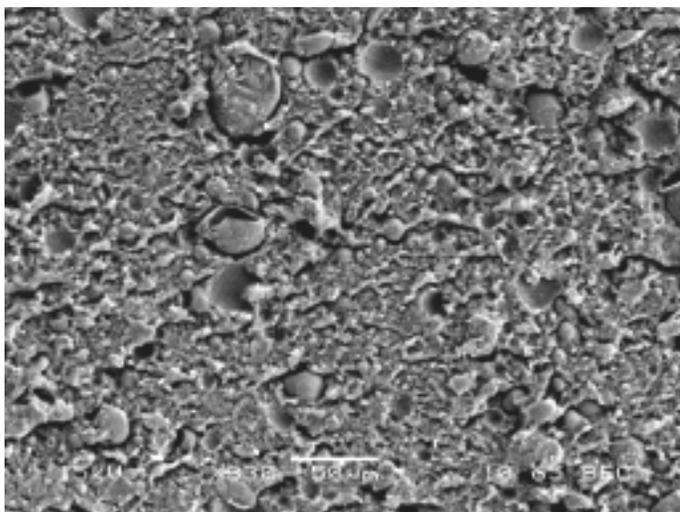


Figure 6. SEM backscattered images of leached samples. Polymer sacs appear devoid of salt and EDS indicates that the matrix phase contains little or no salt, as well: a) sample 15L, b) sample 27H.

While some salt migrates from the interior of the waste form to the surface, the EDS results from Table 3 and the leaching results from Table 4 confirm that at least 10 wt% of salt is encapsulated by the waste form. The micrographs of Figures 3-5 show that the salt is encapsulated as crystals in sacs or corpuscles of polymer embedded in a polymer matrix phase that also contains small salt crystals. These corpuscles may be generated during the mixing process, as the epoxy-PSB emulsion is forming. They become trapped in the polymer phase after the phase inversion occurs. The results of Figure 6 and Table 3 show that the salt is extracted from both the corpuscles and matrix during the leaching of thin sections for long times.

The leaching data of Table 4 confirm that polymer waste forms fabricated using this water-based emulsion flowsheet have good chemical durability. The leachability index measured for each of the samples was in the range of 7.6 to 6.1

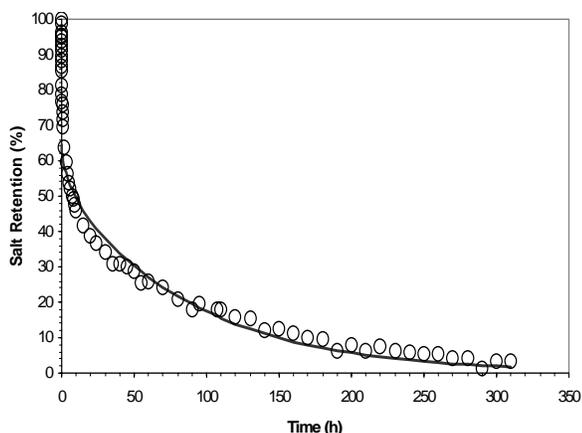


Figure 7. Leaching data for a section of a waste form. The solid line represents a fit of the data with the slab model. The initial fast drop in salt content corresponds to the rapid dissolution of crust salt present on the sample's external surface.

and exceeded the required value of 6. The corresponding diffusion coefficient was in the range of 2.5×10^{-8} to 75×10^{-8} cm^2/s . This range is so low that measurements could only be accomplished by leaching very thin sections of the waste form for long times.

An ideal waste form encapsulates a large amount of waste and prevents the waste from leaching out of the matrix. Attempts to increase the waste loading in the interior of the samples were not successful using the procedures of the current flowsheet. As seen in Tables 2 and 4, samples 20L, 21H, and 27H contain between 10-12 wt% salt in their interior, despite their higher nominal salt loading. In sample 20L, it is likely that large pores form (see Figure 5) because the low liquid content of the sample produces an emulsion that is rather stiff prior to curing. This prevents the emulsion from shrinking as water evaporates during curing, leading to the formation of internal porosity. It is likely that the amount of salt encapsulated by the matrix is strongly influenced by the parameters that control the emulsification and curing processes. More work should be done to determine the influence of the cross-linking agent, surfactant, and curing temperature on waste form properties.

This work has shown that the water-based emulsion process creates waste forms that successfully encapsulate at least 10 wt% highly-soluble salt. When sections of the waste form are subjected to stringent leaching conditions, the measured leachability index for salt meets or exceeds criteria for low-level radioactive waste forms, suggesting that the less mobile toxic metals will meet or exceed the leachability criteria as well. Curing of the waste forms produces a higher concentration of salt in the near surface region than in the interior of the waste form. This analysis indicates that higher salt contents might be achieved if the migration of the solutions towards the sample surface during curing can be controlled.

Nominal wt % Salt	wt % Leached as Salt		Diffusivity (cm ² /s)	Leachability Index, L ₁
	Crust	Interior		
15	1.11	9.89	2.5 x 10 ⁻⁸	7.6
21	3.1	12.4	30 x 10 ⁻⁸	6.5
27	3.2	12.8	75 x 10 ⁻⁸	6.1

Table 4. Diffusivity and leachability index for NaNO₃ in the waste forms. The diffusivities were obtained by fitting the model developed in this work to experimental data. The leachability indices were calculated from equation (8).

ACKNOWLEDGEMENTS

We thank the United States Department of Energy, the National Science Foundation, and Pacific Northwest National Laboratory for giving us the opportunity to participate in the Faculty and Student Teams program. We also thank the Advanced Process and Application Group, especially Loni Peurrung, Bradley R. Johnson, Michael Schweiger and Jim Davis, and the Process Science and Engineering Division within the Environmental Technology Directorate for support this summer. Finally, we thank Royace Aikin, the FaST Program Manager at PNNL, for facilitating the organization of our FaST appointment at PNNL. Our work was completed at the Applied Process Engineering Laboratories (APEL) at Pacific Northwest National Laboratory.

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Abstracts

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BIOLOGY

Cellulose Production by *Gluconoacetobacter hansenii*: Effect of Carbon Source and *Camellia Sinensis* (tea) Extract. SHARON BEETNER (Coe College, Cedar Rapids, IA 52402) JONATHAN WOODWARD (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Cellulose produced by the bacterium *Gluconoacetobacter hansenii* has physical properties different to the more familiar plant cellulose. This bacterium forms a hydrated pellicule or "skin" of cellulose on the surface of the liquid growth media. Native and dehydrated forms of bacterial cellulose have application in biomedical products, environmental remediation, and fuel cell technology. This research studied the synthesis of cellulose by *G. hansenii* under different culture conditions. These included variation of the carbon source, nitrogen source, and growth period. In addition, extracts of teas and hops were added to the medium to investigate the effects on cellulose synthesis. During bacterial growth glucose concentration and pH changes in the media were monitored. Production of cellulose was determined by weighing the mass of the cleaned and dried cellulose. The dried cellulose was also analyzed using Fourier Transform Infrared Spectroscopy to look for other compounds associated with it. The characteristics of the cellulose pellicules were dependent on the culture conditions. Besides glucose, fructose, inulin, mannitol, and galactose were good substrates for *G. hansenii*, but there were significant differences in the weight of the cellulose pellicules produced. *G. hansenii* produced significantly more cellulose when grown on fructose compared with the other sugars tested. Also, cellulose production was dependent on the nature of the growth medium. Extracts of different teas neither inhibited nor stimulated cellulose production but could be used as a sole nitrogen source.

Characterization of MTBE-biodegrading Microbial Communities. AKASHDEEP DHILLON (Fresno City College, Fresno, CA 93741) TAMAS TOROK & DOMINIQUE C. JOYNER (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Under the Clean Air Act Amendments of 1990, fuel oxygenates, such as methyl tertiary-butyl ether (MTBE) have been added to gasoline to increase combustion efficiency and reduce air pollution. MTBE is a soluble soil and groundwater contaminant that gives an offensive smell and taste to the drinking water. Researchers have been identified microorganisms that co-metabolize MTBE. At the Center for Environmental Biotechnology at LBNL, two fluidized bed reactors filled with granulated activated carbon are supplied with water containing MTBE at concentration of 45-60mg/l. One of the reactors was inoculated with an enrichment culture that was fed with 2-methyl butane. In the other reactor an endogenous microbial community has developed. Both reactors have shown successful MTBE biodegradation for over 300 days. The current research reports on the use of molecular-level microbiology tools for the characterization of the microbial communities in the MTBE treatment reactors to complement other means of reactor performance characterization. Scanning electron microscopy (SEM) of activated carbon particles indicated the presence of diverse microbial communities in the reactors. Fatty acid methyl ester (FAME) analysis suggested that there were changes in the microbial community structure over time. This observation correlated with changes in MTBE treatment in the reactors. Terminal restriction fragment length polymorphism (t-RFLP) analysis is in progress to further evaluate the genetic diversity of the microbial communities within the two MTBE treatment reactors.

Identification and Characterization of Intergenic Suppressors in Sporulation Temperature-sensitive Mutants of *Bacillus subtilis*. JESUS HERNANDEZ RIVERA (UPR-Mayaguez, Mayaguez, PR 00676) TERRANCE LEIGHTON (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The characterization of intergenic suppressors in *Bacillus subtilis* is a powerful tool to identify which cellular components control the bacterial sporulation process. In *Bacillus subtilis*, the isogenic strain, W168, is able to sporulate at non-permissive temperature (47°C). However, isolated strains with L17 and L22 ribosomal protein mutations are resistant to several antibiotics, and were characterized oligosporogeneous at non-permissive temperature (spots). An intergenic suppressor called the rev mutation was able to suppress the spots phenotype and was located in an unknown locus nearby the spo0F region. A gene walking strategy coupled with sequencing

analysis revealed that the mutations named rev 4, 10 and 11 were located at positions 341bp, 751bp and 343bp of the rho gene respectively. It was hypothesized that Rho may be implicated in the regulatory mechanism of sporulation genes. Rho is involved in gene transcription termination in gram negatives but it has no known function and is considered inessential in *Bacillus subtilis*. RT-PCR of selected sporulation genes on W168, spots mutants and rev mutants suggests that Rho may have a role in the sporulation process. These results revealed a different expression pattern of sinI, which is an inhibitor of the sporulation repressor sinR. To confirm Rho involvement in the sporulation process, a deletion plasmid vector was constructed to knock out the rho gene from Spots mutants. Transformation of the deletion vector in *Bacillus subtilis* will be performed and the sporulation frequency will be determined. A difference in the sporulation frequency should be seen, suggesting that rho regulate sporulation genes.

Modeling RNA Double Helical Structures of Arbitrary Sequence. ALAN HILLSTEAD (Southern Utah University, Cedar City, UT 84720) STEPHEN R. HOLBROOK (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The growing body of genomic information has led to an increase in the need to develop algorithms and computational methods to sort and utilize the data. Among algorithms there has been some work with those that point to the possibility of modeling three-dimensional structure of biological molecules. Previous methods for producing RNA helical structures have been limited to producing only canonical structures incapable of incorporating mismatched (non Watson-Crick) base pairs. We have developed a method for producing RNA double helical structures of arbitrary sequence. The method builds a new helical structure file using experimental data collected and stored in databases such as PDB and NDB. The method has proven to be efficient in creating files unconstrained by the limitations of base pairing and canonicity. Early preliminary comparisons yield promising results that indicate that the algorithm improves the accuracy of current methods in producing RNA helices that mirror experimentally resolved molecules.

Search for Ultraviolet-A Induced DNA Damage in Melanin-containing Human Cells Utilizing *Schizosaccharomyces pombe* UVDE Endonuclease. TSUHAO DAVID YEUNG (University of Rochester, Rochester, NY 14627) RICHARD B. SETLOW (Brookhaven National Laboratory, Upton, NY 11973).

It is known that the UVB waveband (280 - 320 nm) has the capability to induce DNA damages, such as cyclobutane pyrimidine dimers, while the effects of UVA (320 - 400 nm) remain relatively mysterious. If not repaired, these damages negatively affect the cell's homeostatic functions and abilities to replicate and differentiate, resulting in cell death and cancerous growth. In our studies, we used UVDE endonuclease, isolated from *Schizosaccharomyces pombe*, and alkaline gel-electrophoresis to attempt to identify UVA-induced damages occurring in pigmented melanocytes after exposure to UVA wavelengths over 320 nm, using UVC (254 nm) exposure on pUC18 plasmid DNA as a positive control. Our preliminary results indicate the need to use a different UV-endonuclease, as UVDE failed to distinguish the presence of UVA-induced adducts.

Biochemical Characterization of XPG Associated Protein 1, XAP1. MICHAEL ZUNDEL (Southwestern College, Chula Vista, CA 91910) PRISCILLA COOPER (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Xeroderma pigmentosum (XP) is an inherited nucleotide repair disorder arising from a mutation in one of seven genes (XPA-XPG). Patients afflicted with XP exhibit a dramatic >1000 fold increase of UV-induced skin cancer due to a break down in the mechanisms that repair DNA damage caused by UV radiation. XPG is a 3' endonuclease involved in many facets of DNA repair, including Nucleotide Excision Repair (NER) and Transcription Coupled Base Excision Repair (TC/BER). A previously unknown protein was identified by mass spectrometry after specific co-immunoprecipitation with XPG and named XAP1, for XPG-Associated Protein. XAP1 is predicted to encode a protein of 2089 amino acids with a forkhead-associated (FHA) domain at its N-terminus, a central region with 18 tandem repeats and a BRCA1 C-terminal (BRCT) domain at its C-terminus. In order to elucidate the structure and function of XAP1, fragments of the N-terminus, C-

terminus, a central helical domain, and the repeat domain were subcloned into pET vectors. The fragments were expressed in *E. coli* using IPTG-inducible promoters. The recombinant proteins were tagged with a 6xHis tag for western blotting analysis and for ease of purification. Purified protein, obtained via nickel affinity column purification, will be used to raise antibodies against XAP1 for immunological studies and for structural crystallographic studies. Identifying the structure and function of this novel protein XAP1 will help to better understand the intricacies of DNA repair and the maintenance of genomic stability.

Participation of src Gene in Cadmium-induced Bone Changes in Mice. ADETOWUN ALIMU (*Malcolm X College, Chicago, IL 60612*) MARYKA BHATTACHARYYA (*Argonne National Laboratory, Argonne, IL 60439*).

Cadmium is a heavy metal known to have an adverse effect on people exposed to it both in environmental and occupational settings. We hypothesize that cadmium acts by stimulating osteoclastic pathways to release calcium-45 from bone. Mice heterozygous for src gene deficiency were mated and produced a litter of four heterozygous wild type pups (+/0= +/+, +/-). Mother (dam) was administered calcium-45 drinking water for skeletal labeling. Calcium-45 was transferred to pups through breast milk during lactation. The pups were weaned into metabolism cages with powdered basal diet where fecal and urine collections were made. Two doses of cadmium solution were given by gavage, one on day 25 and the second on day 32. Fecal and urine collections were dissolved in hydrochloric acid and placed into a scintillation counter to determine amount of calcium-45 excreted in feces and urine. Upon analyzing the data, cadmium targeted the bone to cause a slight increase in fecal calcium-45 concentration of mice that received cadmium doses compared to the control mouse. These results show that cadmium on exposure acts on bone to cause the release in the calcium content of src normal mice (wild type). This experiment provided a mouse model to study the effect of cadmium on the release of calcium from bone in src or fos gene deficient mice.

Parvovirus B-19 Phospholipase A2, Purification for Crystallization and Structure Determination using X-Ray Scattering. RAMON ALLENDE (*Central del Caribe School of Medicine, Bayamon, PR 00960*) MARC ALLAIRE (*Brookhaven National Laboratory, Upton, NY 11973*).

Parvovirus B-19 is a virus member of the Parvoviridae family that infects human cells. It has been shown that the capsid of this virus carries a phospholipase (PLA2), which is crucial for the infection process. The goal of this project is to crystallize the protein in order to elucidate its three-dimensional structure using X-Ray crystallography. To carry out crystallization experiments the protein needs to be pure (95%+). This was achieved using proteases and FPLC methods. At this point the protein is in a pure state. Current experiments include screening for crystallization techniques to determine the optimum crystallization parameters of the protein. Eventual success of these experiments will help understand in detail the infection process and will aid in the development of specific antiviral agents for the active site of PLA2.

Remote Sensing: Development of a Field Protocol for Measuring Leaf Area Index (LAI) With an Optical Instrument. VONEKIA ATKINSON (*Jackson State University, Jackson, MS 39217*) ROBERT WASHINGTON-ALLEN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Remote sensing refers to gathering information from an object without being in direct contact with that object. The purpose of my research was to develop a field protocol for using the LI-COR LAI 2000, a remote sensing instrument that measures radiation transmittance through canopies. The LAI 2000 measures the leaf area index (LAI, m²/m²) of plant canopies, a measure of canopy structure. This optical instrument consists of a light wand, viewing caps ranging from a 30 degree to a 360-degree field of view (no cap), and a data logger. The initial protocol consisted of 23 steps in a flow chart that showed the operator how to operate every aspect of the instrument. This protocol was too detailed and was reduced to a shorter final protocol that led the operator through 19 steps and was developed to be "dummy proof". The final protocol was a general list that is more suitable for an operator in the field. The final protocol was easier to follow and contained the exact information needed for making LAI measurements including flexible sampling schemes for both different vegetation cover

types, e.g., woodland as opposed to grassland, and spatial configurations, e.g., linear rectangular woodland hedgerows, square pastures or hayfields.

Stable Isotope Labeling by Esterification for the Selective Enrichment and Isolation of Phosphopeptides Using IMAC Chromatography. MEGAN BRUEMMER (*Whitman College, Walla Walla, WA 99362*) DAVID CAMP (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Phosphoproteins and the process of reversible phosphorylation are responsible for almost all aspects of cellular function. Analysis of phosphoproteins begins at the peptide level, yet isolation of phosphopeptides can be challenging. A primary goal of this research was to develop a method to determine the ratios between common phosphoproteins in MCF7 strains Clone-18 and Neo cells. Such understanding would help target areas to concentrate breast cancer research. The first step in the enrichment method was to modify the peptides by esterification. This prevented non-specific binding to enrichment method of immobilized metal affinity chromatography (IMAC), and avoided the need for low pH. The designed method was tested on beta-Casein with analysis by liquid chromatography and tandem mass spectrometry. Results show that the esterification chemistry worked completely, and that the enrichment method was effective for a single protein. Before the MCF7 strains could be tested on the new phosphopeptide enrichment column, stable isotope labeling was used to differentiate between the two strains. Clone-18 was esterified with methanol, while Neo was labeled with deuterated methanol. The samples were combined in equal amounts so the intensity of their peaks would indicate their abundance ratio. The d0/d3 labeling method worked with relative accuracy with beta-Casein, but insufficient results were obtained from the MCF7 peptides to make any definite conclusions. The IMAC column approach will need to be altered in order to enrich for phosphopeptides in a more complex matrix.

Overexpression and Purification of Integral Membrane Proteins P10 and P11. MAUREENE CARDENAS (*Manhattanville College, Purchase, NY 10577*) ANAND SAXENA (*Brookhaven National Laboratory, Upton, NY 11973*).

The integral membrane proteins, P10 and P11, were studied to understand their protein functions and importance in vivo with relation to the electron transport chain and expression during glucose deprivation respectively. The protein samples were isolated, solubilized in urea, purified, and eventually crystallized using various techniques. Both dialysis and size exclusion chromatography were used in order to obtain a pure sample with minimum DTT and detergent. Results indicated that P10 was easily solubilized in urea while P11 was not. Dialysis output was reduced five fold to what was initially inserted for both protein samples. Size exclusion chromatography indicated that the P10 protein sample eluted out at a level and time between both BSA and cytochrome c standards. P11 has yet to be tested using the size exclusion column, but it is believed that it will follow the same path as the P10 sample. In completing the experiment the protein sample will be crystallized and then analyzed using atomic resolution using protein crystallography diffractometers at the National Synchrotron Light Source at Brookhaven National Laboratory.

Characterization of a Xiphophorus Backcross After Exposure to UV Light. MICHELLE CARLEY (*Cornell University, Ithaca, NY 14850*) RICHARD SETLOW (*Brookhaven National Laboratory, Upton, NY 11973*).

The incidence of melanoma, the most serious form of skin cancer, has more than doubled in the United States in the past 20 years. Sunlight, especially in the UV range, is commonly implicated. Interspecific backcrosses of the tropical fish *Xiphophorus* are susceptible to melanoma resembling human melanoma after exposure to UV light and have been used as a model for human cancer for decades. To study the effects of certain ranges of light on melanoma induction in our hybrids, backcross hybrids were exposed to an intense UV irradiation at 7 days old and grown to 6 months. They were sacrificed and preserved for future histological examination.

A Proteomics Approach to Studying Glycosylated Membrane Proteins. SHERENE CARTER (*Idaho State University, Pocatello, ID 83201*) DEANNA AUBERRY (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Many glycosylated membrane proteins, such as Epidermal Growth Factor Receptor (EGFR), are responsible for triggering cell growth. They are possible biomarkers for cancer research, but difficult to study because of their amphipathic structure. They are also found in relatively low abundance in a cell. A directed proteomics approach has been used to separate glycosylated membrane proteins from the thousands of others in human ovarian cancer cells. Digestion, separation of peptides, and mass spectrometry were the analytical techniques performed to determine protein enrichment. Cell lysis and solubilization followed by lectin chromatography was a successful procedure for enriching glycosylated membrane proteins.

Differential Detection of the Potyviruses: Potato Virus Y and Tobacco Etch Virus Through the Use of a Biochip Assay. LAVEDA CASTERLOW, JASMIN FEIMSTER, and RAKISHA NICHOLASON (North Carolina Agricultural and Technical State University, Greensboro, NC 27411) DARRELL CHANDLER (Argonne National Laboratory, Argonne, IL 60439).

Through the use of a biochip, viral pathogens of the plant family Solanaceae including species of pepper, tobacco, tomato, and potato will be detected. Oligonucleotide sequences specific for Potato Virus Y (PVY) and Tobacco Etch Virus (TEV) were placed on the biochip. Using the National Center for Biotechnology Information website, primers for the seven viruses were selected and were used to generate probes. Capsid protein regions of each virus were blasted against those in the database. Those regions found in the database were placed into ClustalW software to align the nucleotide bases. Information was gathered using the Serpntn software to detect similarities amongst the viruses and provide the primers, which will serve as the template on the biochip. Only perfectly aligned oligonucleotides with fifty base pairs could be blasted into the NCBI software to ensure that the desired virus was the only plant virus obtained from that blast. Group and specific 20mers in the 5' to 3' direction were obtained by a blasting procedure that was specific for a particular isolate or group of isolates. All 20mers were then placed in the ClustalW window and aligned to make certain that each 20mer was specific for a particular group, strain, or virus. Each 20mer was then translated using Chargaff's rule and reversed to create 3' to 5' probes. The probes were placed into a table that consisted of accession number, type of protein (capsid or replicase), strain/isolate, location, melting temperature, and 20mer sequence.

Protein Production for Structural Genomics Project. POLY CHAN (Harry's Truman College, Chicago, IL 60440) SHIU MOY (Argonne National Laboratory, Argonne, IL 60439).

The structure and function of proteins is a continuing research that concerns scientists all over the world. The Humane Genome Project, which mapped out all the genes of the human body, has been accomplished. Currently scientists are interested with the structure and functions of those particular genes. Scientists understand that genes in a specific order develop into proteins and proteins are needed in order for our bodies to function correctly. For example, proteins are responsible for oxygen transport by hemoglobin from lungs to muscle cells, antigen which binds to an antibody that protects against disease agents, cells surface which transports food molecules into a cell, structural proteins which maintain the physical form of vertebrates includes the following extracellular varieties: elastin, and keratin; Collagen makes up about 25% of the proteins in humans which is a connective tissue found in ligaments, and muscle coverings called sarcomeres; Keratin is an intracellular protein forming the layer of dead skin cells; It is however found extracellularly as hair, birds, claws or most mammals. In other words, proteins are important in order for humans to exist. This research paper focuses on the steps of manual work on the process of transformation, expression, and solubility of proteins. The results obtain are protein samples that were successfully expressed and soluble.

The Effects of CAGERS on Nuclear Intracellular Inclusions in Huntington's Disease. WAI KAN CHIU (University of California at Berkeley, Berkeley, CA 94720) YOSHINORI KOHWI (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The group of Kohwi discovered neuronal mRNA binding proteins, CAG Element Recognizing proteins (CAGERS) that bind single-stranded (CAG) and (CGG) repeats. To study a link of CAGERS to trinucleotide repeat disorders, the Kohwi's lab employed Huntington's Disease (HD) model mice (R6/2) and established double transgenic (tg) mice carrying

CAGER-1-tg in HD-tg mice. HD is an adult-onset neurodegenerative disorder expressing an expanded (CAG)-repeat in the huntingtin gene. The Kohwi's lab found that the phenotype of HD was characterized by an earlier onset and a stronger clasping reflex in the double-tg mice compared with that of HD-tg mice alone. Some CAGER-1-tg/HD-tg double transgenic mouse lines had a much shorter life span than that of the HD-tg mice. By contrast, HD-tg in the CAGER-2-Knockout mice resulted in a prolonged life span compared with that of HD-tg mice alone. In this summer program, I have analyzed those double tg mouse brains from the point of neuropathology employing specific antibody against aggregated mutant huntingtin in nuclei (Nuclear Intracellular Inclusions, NIIs) by immunofluorescence. One characteristic of HD is the formation of NIIs in striatum and cortex, where severe neurodegeneration takes place, suggesting that NII formation pathway is central of molecular pathology of HD. We found that NIIs were formed in 8-week-old CAGER-1-tg/HD-tg mice but not in the same age HD-tg mice. Our data show that CAGERS' expression in neurons modulates the onset of the disease phenotype, neuropathology, and the life span of the HD in the model mice.

Evaluation of the Gateway™ Cloning Technology for Shewanella oneidensis MR-1 Cytochrome, Sensor and TAT Genes into pET-DEST42TM. STEPHANIE CHU (University of California, Davis, Davis, CA 95616) MARGIE ROMINE AND G. NEWTON (Pacific Northwest National Laboratory, Richland, WA 99352).

The Gateway™ Cloning Technology holds promise for rapidly constructing different types of fusions to a single gene. Once an initial "entry" clone is constructed from a PCR product, it can be used to construct many different fusion clones by recombinase activities rather than slow traditional cloning techniques that rely on restriction digestion and ligation. Using this system we constructed 15 "entry clones" and successfully transferred 12 of the inserts into a secondary vector that results in fusion of poly-histidine to the c-terminus of the gene. We found that the most time consuming processes of the Gateway™ Cloning Technology was in generating the PCR product for cloning into the entry clone. Furthermore, we found that we could halve the amount of recombinase reagent necessary to produce the his-fusion clones, thereby, greatly saving cost on the process. The his-fusion clones constructed can be used to purify protein for protein-protein interaction studies, antibody production, and Raman analysis. The entry clones can be used to rapidly generate other types of fusions (i.e., green and yellow fluorescent protein) for electron and atomic force microscopic imaging of bacteria expressing these fusion proteins so that we can monitor their localization and activity within *S. oneidensis* cells.

Structural Analysis of Native Membrane Proteins and Expression of Foreign Membrane Proteins in Rhodospirillum rubrum sphaeroides. ADAM CRAWFORD (Ripon College, Ripon, WI 54971) PHIL LAIBLE (Argonne National Laboratory, Argonne, IL 60439).

Membrane proteins, while integral components of cellular processes, are limited in terms of knowledge about their structures because of difficulties that arise when isolating and purifying these proteins in preparation for structural and functional analysis. The structure of the membrane-bound photosynthetic reaction center (RC) of Rhodospirillum (R.) rubrum sphaeroides has been determined by molecular replacement, a technique in which phases are determined by comparison of similar X-ray diffraction patterns of previously solved proteins. This particular structure has yet to be determined by isomorphous replacement, in which introduction of a heavy atom in a protein crystal determines the phases by causing diffraction pattern changes relative to a crystal without the heavy atom substitution. In my research, RCs with the heavy atom derivative selenomethionine incorporated in its amino acid chain were crystallized and used by staff crystallographers to determine unique experimental phases and unmatched electron density maps of the R. rubrum sphaeroides photosynthetic reaction centers. Success of Argonne's Rhodospirillum expression system with respect to native proteins has suggested that the system can be used for expression and purification of foreign proteins as well. In another aspect of my research, efforts were made at expression in Rhodospirillum of eight membrane proteins from the syphilis causing spirochete, Treponema (T.) pallidum.

Phylogenetic Characterization of Environmental Isolates Using Ribosomal RNA Sequence Analysis. JOSHUA CURRIE (Tennessee Technological University, Cookeville, TN 38501) TAMAS TOROK (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

In the last twenty years, environmental microbiology has undergone a revolution of new and innovative molecular biology techniques. Perhaps the most overwhelming discovery of this molecular revolution has been the realization of how few organisms have been identified and how little is understood of microbial ecological dynamics. This vast resource of uncharted microorganisms coupled with new molecular tools such as rRNA sequence analysis have yielded the identification of new taxa, many of which present the potential for applications in industry, agriculture, and medicine. Seven eukaryotic organisms were phylogenetically characterized by 18S rRNA sequencing. Sequence data was submitted as queries to online databases to align the samples with known organisms. Phylogenetic inference was used to construct phylograms of the organisms as they related to each other as well as to classified eukaryotic species. All seven samples were linked to the fungal Order Ascomycetes with evolutionary similarity to many species that are well recognized for their beneficial attributes or pathogenicity. Although a definitive identification could not be made, phylogenetic characterization has provided a tool for assessing which samples are good candidates for further characterization of morphology, metabolism, and reproductive cycles using traditional microbiology techniques.

Pharmacodynamic Responses of Target Tissues Exposed to Various Concentrations of the Organophosphate Insecticide Diazinon in Rats. STEPHANIE DENNISON (University of Maryland Baltimore County, Baltimore, MD 21250) CHARLES TIMCHALK (Pacific Northwest National Laboratory, Richland, WA 99352).

Diazinon is a thionophosphate pesticide that when metabolized into its oxon, competitively inhibits cholinesterases. In order to develop a physiologically based pharmacokinetic and pharmacodynamic (PBPK/PD) model for the organophosphate insecticide diazinon (DZN) in rats, a quantitative investigation of the pharmacodynamic response associated with acetylcholinesterase inhibition in targeted tissues of the body, namely the brain, blood, and diaphragm, is needed. Using a spectrophotometric assay (Ellman et al., 1961), the extent of esterase inhibition following orally administered diazinon in corn oil at doses of 100 mg and 50 mg DZN/kg body weight over a 24-hour time course provides insight to the inhibition and recovery of acetyl- and butyrylcholinesterases in vivo. When comparing the 50 mg and 100 mg DZN/kg body weight time course of each tissue, little difference was seen between the degrees of inhibition at each dose. This was consistent with the plasma, red blood cells (RBCs), brain, and diaphragm. The extent of inhibition followed the pattern of plasma>RBCs>diaphragm>brain. This was expected due to the method of dosing, and anticipated distribution of diazinon determined by blood flow, partitioning, and concentration of cholinesterases in the tissue. This work is a small portion of a much larger project being researched to develop a PBPK/PD model for diazinon in the rat, as well as investigate PBPK/PD model interactions for organophosphate insecticides in rats and humans.

Characterizing Microbial Communities of ex-situ Bioreactors using Molecular Techniques. AKASHDEEP DHILLON (Fresno City College, Fresno, CA 93741) TAMAS TOROK (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Molecular techniques that are traditionally used to characterize isolated pure strains were used on microbial communities of ex-situ bioreactors to monitor the structure and diversity of microbial communities in the bioreactors. Three reactors of interest were sampled: two fluidized bed reactors capable of MTBE degradation and a nitrifying reactor. Samples were taken monthly from the two FBR reactors and bimonthly from the nitrifying reactor to observe the change in microbial community structure and diversity over time. Techniques such as FAME and t-RFLP were applied over time on samples from all three reactors to observe microbial communities. SEM images were taken of activated carbon particles from MTBE reactor and they indicated the presence of a diverse microbial community on the activated carbon particles. FAME and t-RFLP analyses suggested that the microbial community structure changed over time and in response to changes in chemical feed to the reactors. These findings correlated with chemical changes in the MTBE treatment reactors upon addition of gasoline. Both FAME analysis and t-RFLP analysis showed expectedly stable communities in the nitrifying reactor with no change in the reactor conditions. It can be concluded that these techniques are reliable tools for the observation of structural or diversity changes of communities over time. Another DNA-based technique 16S rRNA gene sequencing

of pure isolates from the MTBE reactors is in progress.

Protein Crystal Growth: Trials and Errors. MARIA DISS (University of Puget Sound, Tacoma, WA 98416) VIVIAN STOJANOFF (Brookhaven National Laboratory, Upton, NY 11973).

The vapor diffusion technique for crystallizing proteins has become one of the most widely used methods of crystallization. Many factors influence the crystal growth within this method. To our knowledge there has been no systematic study to compare the different techniques and configurations. The purpose of this study is to compare the various methods of vapor diffusion used in crystallization. Hen egg white lysozyme (HEWL) was employed as the test protein. The same experimental conditions such as protein concentration, pH, temperature, purity and reservoir solution volume were maintained through all assays. The use of various salts (NaCl, MnCl₂, NiCl₂ and ZnCl₂) as a mean to further crystallization and oil (mineral oil and glycerol oil) as a mean to control the diffusion rates were investigated. The experiment confirmed that anions are more effective than cations as salting out agents. Nucleation was not slowed significantly with the use of mineral oil. However, glycerol oil had an important effect on crystal growth.

Bioconversion and Desulfurization of Heavy Oil with Mixed Microbial Cultures. APRIL DUFFY (Community College of Rhode Island, Warwick, RI 02886) MOW S. LIN (Brookhaven National Laboratory, Upton, NY 11973).

Fossil fuels are being used for power generation and in the chemical industry at an increasing rate. Standard regulations pertaining to atmospheric emissions require reduced levels of sulfur oxides as by-products of oil and other fossil fuel use. Concurrently, methods of bioconversion and desulfurization of heavy crude oils are being researched. Microbial cultures are inoculated, incubated, and monitored for growth in mixtures of mineral medium and heavy oil. Samples are analyzed qualitatively and quantitatively using Gas Chromatography-Mass Spectrometry (GC-MS). The GC-MS analyses provide confirmatory information regarding the success of microbes in bioconversion.

Cancer in Invertebrates. JAMES EDWARDS (Contra Costa Community College, San Pablo, CA 94806) JUDITH CAMPISI (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

My task was to research the evolution of cancer. It is known that basically all vertebrates get cancer. It was my assignment to find out which invertebrates were also susceptible to cancerous growth. I identified as many taxa as I could for which there is evidence of tumors, and kept track of what sort of tumors those were. For my particular research cancer was defined as any abnormal cell proliferation in an ADULT organism. I theorized that cancerous cells evolved at the same time that regenerating cells came into being. Therefore, hemimetabolous insects would be prone to have cancerous cells, while homometabolous insects wouldn't. To collect my data I read a vast amount of journals and literature that pertained to this study. At the end of my research, I found my theory to be inconclusive. Both hemimetabolous and homometabolous insects proved to be capable of housing cancerous cells. In addition to insects, various arthropods, echinoderms, mollusk, sipunculida, platyhelminthes, and annelids were also found to have cancerous cells. From the data collected it can be assumed that some organisms have some sort of tumor-suppressing mechanism so that they are resistant to cancer. It is also clear that many invertebrates clearly have irregular growths that can be considered cancerous. The research is still in progress and eventually want to find out how tumor-suppressing evolved and came into being.

Transgenic Medaka Embryos as a Bioassay for Mutagen Containing Sediments from Long Island Sound. SEBASTIAN GALASKA (Housatonic Community College, Bridgeport, CT 06604) RICHARD SETLOW AND LYNN MENDELMAN (Brookhaven National Laboratory, Upton, NY 11973).

Years of declining lobster and other sea harvest have increased the concerns of what is going on in the surrounding environment. Pesticides and chemicals (run off) being released into areas such as the Long Island Sound are thought to be significant factors in their declining health. These chemicals have potentially adverse effects on the wild life, the industry that relies on this wild life, and humans on which the impact is still unrealized. The medaka fish (*Oryzias latipes*) model is used to test the dose response rates of two known mu-

tagens, Benzo[a]pyrene (BaP) and 7H-diBenzo(c, g)carbazole (DBC), so as to assess the suitability of these fish as a model. By exposing the embryos to sediments containing a prepared concentration of these chemicals, concentrations that should produce mutations, yet still allow the embryo to survive and develop, can be obtained and used in further studies. Embryos were placed on sediment containing, either DBC or BaP at concentrations of 56, 166, 500, 1500 ug/g (dry weight). The results showed that the concentration of the chemical was not a major factor in the hatching of the fry. The amount of mutations that occurred is still pending analyses. They also showed that there are a large number of variables with fish and embryos. For example, the temperature and water quality must be kept constant or things like fungal contamination will greatly reduce the viability of the embryos.

Strobe Light Deterrent Efficacy Test at Grand Coulee Dam Third Powerplant Forebay — Preliminary Analysis. LODA GRIFFETH (University of Alaska, Fairbanks, Fairbanks, AK 99775) ROBERT L. JOHNSON (Pacific Northwest National Laboratory, Richland, WA 99352).

In a recent study conducted by the Colville Confederated Tribes, it was determined that between 200,000 and 600,000 fish from Lake Roosevelt were entrained in the turbines at Grand Coulee Dam. Approximately 85% of the fish passed through the dam's third powerplant. Due to the importance of the fishery and severity of the problem, a three-year pilot study began to test the phototactic response of fish, specifically kokanee (*Oncorhynchus nerka*), land-locked sockeye salmon, and rainbow trout (*Oncorhynchus mykiss*), to light intensities produced by strobe lights in the third powerplant forebay. Splitbeam hydroacoustics was used to monitor the efficacy of the light treatments and fish behavior. Preliminary analysis revealed that during night treatments, the ambient light levels were near zero allowing the effects of the strobe light treatments to be observed. Based on manually tracked fish targets, approximately 75% of the fish targets (587 out of 783) were observed at night. Over 60% of those fish targets were detected during the application of the three strobe light configurations. Preliminary analysis suggests that light intensities for the two "lights on" treatments invoked a phototactic response from fish. Further analysis of data will determine whether fish response was positive or negative to each individual treatment.

Identification of Biochemical Pathways using Petri Nets. DEAN GULL (Southern Utah University, Cedar City, UT 84720) JANET JONES-OLIVEIRA (Pacific Northwest National Laboratory, Richland, WA 99352).

A computational model has been developed which accurately depicts pathways of enzyme-catalyzed reactions as specialized directed graphs. This graphical model is a first step toward a goal of facilitating manipulation and study of a complete biochemical system. Petri net representations of biochemical reactions are specific and detailed. In modeling a biochemical pathway with a Petri net, places represent an organic chemical species, transitions represent a chemical event. Minimal cycles, within the Petri net, identify where flux conservation is being achieved. Understanding the flux of a system can lead to the manipulation of feedback; thereby controlling the overall productivity of the network.

The Genomic Sequencing and Cross Species Comparisons of the PPAR-Gamma Gene. MICHAEL HAMAGUCHI (Merced College, Merced, CA 95340) JAN-FANG CHENG (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Many common species share similarities throughout portions of their genomes. In the case of this specific gene PPAR γ , Peroxisome-Proliferator-Activated-Receptor-Gamma, comparisons can be made among a large variety of classes not only mammalian species. However for this comparison three differing classes have been observed: Rabbit, Opossum, and Chicken. The process starts with the generation of subclone libraries for each BAC size (100-200kb) genomic interval then those colonies are deposited into well plates where they then get amplified, primed, and eventually sequenced. Once enough information is gathered, software aided statistical comparisons are made between exons, untranscribed regions, and conserved noncoding regions of the genomic intervals. The results mainly highlight the conserved noncoding genomic regions between the corresponding genomic intervals and show us where regions have remained virtually identical for tens of millions of years if not

hundreds. The PPAR γ gene seems to have a variety of roles in the body, which vary among population as well as tissue type and dietary habits. The protein encoded by PPAR γ gene is currently being studied for its effect on type 2 diabetes, obesity, atherosclerosis, and cancer. By targeting PPAR γ researchers have established that the gene is involved in glucose and lipid homeostasis/differentiation. The targeting of PPAR γ gene has been shown to have a stunning effect on cancers of the breast, prostate, and colon. PPAR γ promotes terminal differentiation of the malignant epithelial cells in the breast and can severely inhibit the growth of prostrate adenocarcinomas.

Germination Enhancement of *Oenothera pallida*. JENNIFER HESTER (North Idaho College, Couer d'Alene, ID 83814) MICHAEL R. SACKSCHEWSKY (Pacific Northwest National Laboratory, Richland, WA 99352).

Enhancing our knowledge of *Oenothera pallida* (pale evening primrose) germination requirements under laboratory conditions enables us to better understand and potentially improve the germination success of this species in its natural habitat. Previous laboratory experiments for this species have resulted in low success. *Oenothera pallida* is a perennial forb native to dry, shrub-steppe environments. Special emphasis was placed on growing conditions of the Hanford area due to the Department of Energy's attempt to increase plant species diversity in its restoration projects. Petri dishes consisting of fifty seeds each underwent a fully replicated (x3) control, potassium nitrate (KNO $_3$) treatment, and a soap treatment in two temperature, light, and substrate regimes. The KNO $_3$ treatment consisted of watering the seeds with a 0.2 percent KNO $_3$ solution while the soap treatment similarly entailed watering the seeds with an alconox soap solution. The control used water only. The seeds were examined daily for germination and moistened as needed. Findings show that germination was significantly effected by temperature ($p < 0.0001$), watering solution ($p = 0.0048$), and the interaction between temperature and solution type ($p = 0.0004$). The KNO $_3$ treatment did not appear to enhance germination. Further experimentation involving different temperatures may enhance germination success.

The Role of Mitogen Activated Protein Kinase Pathways in the Shedding of Tumor Necrosis Factor Alpha and its Receptors.

ROCHELLE HINMAN (Whitworth College, Spokane, WA 99251) BRIAN THRALL (Pacific Northwest National Laboratory, Richland, WA 99352).

Tumor necrosis factor alpha (TNF- α) is a trigger protein for signaling pathways within the body. TNF- α is linked to a variety of physiological and pathological conditions, including rheumatoid arthritis and type two diabetes. The cytokine is a part of the body's response to infection and is capable of inducing inflammation. On a cellular level, TNF- α is involved in both apoptosis and the transcription of genes essential to cell survival; two seemingly opposing processes. This study focuses on the shedding of TNF- α and its associated receptors in a murine macrophage RAW 264.7 cell line. The relationship of the mitogen activated protein kinase pathways ERK and p38 to observed shedding is of particular interest. The ERK pathway is related to cell proliferation whereas the p38 pathway is more commonly associated with cell stress and apoptosis. The stronger involvement of the ERK pathway in observed shedding of TNF- α and tumor necrosis factor receptor 2 (TNF-RII) indicates that such shedding is a protection response.

The Effect of Cadmium on the Calcium Content of Src Deficient Mice. SARITA HOEKZEMA (Hope College, Holland, MI 49422) MARYKA BHATTACHARYYA (Argonne National Laboratory, Argonne, IL 60439).

Cadmium has been found to increase the break down of bone by increasing the number of osteoclasts found within the bone in cell culture. Src deficient mice have osteoclastic cells but are found to be inactive. Using this information an experiment was designed to see whether cadmium could increase the breakdown of bone in the src deficient mouse. Mice known to be heterozygous for the src gene were bred. When pups were produced, a solution of calcium-45 water was given to the dam to label the pup's skeletons. The pups were weaned into metabolism cages where fecal and urine collections were made. A cadmium solution was administered by gavage on day 25 and 32. The fecal and urine collections were dissolved and placed into scintillation vials and counted within a scintillation counter to determine calcium concentration. After analyzing the results, it was found that a response to cadmium could be seen as a slight increase in fecal calcium concentration for animals receiving the cadmium gavage

compared to a downward trend in the control. This difference follows our hypothesis for this experiment thus showing that cadmium caused an increase in the amount of calcium excreted from the body. Although the first round of breeding produced only wild-type mice, this experiment developed a protocol that is going to be used for follow-on experiments testing the same hypothesis with src-deficient mice.

Electron Microbeam Studies of Micronuclei Formation in Normal Human Diploid Fibroblasts. BROOKE HOLBEN (*Washington State University, Pullman, WA 99163*) MARIANNE SOWA RESAT (*Pacific Northwest National Laboratory, Richland, WA 99352*). Currently the standards for human exposure to ionizing radiation are set by extrapolating the data obtained in the high dose regime to the low dose regime. Historically it has not been possible to provide quantitative data under low dose conditions because the biological responses are below the standard detection limits. Using a spatially resolved single cell irradiator, we are seeking to understand the biological consequences and health effects associated with very low doses of low LET irradiation. The device utilizes a pulsed energetic electron beam that is directly interfaced with a biological sample. The resolution is such that we can selectively irradiate individual cells. In these sets of experiments, we have begun to explore the chromosomal damage yielded by low-LET ionizing radiation on human diploid fibroblasts (AG01552) using a micronuclei assay. Preliminary data is presented which demonstrates the need for the use of cells at low passage numbers to maintain low background levels of micronuclei. Using a ⁶⁰Co source we obtained preliminary data on the dependence on percent of micronuclei versus the number of days incubated post irradiation. A dose response curve for an initial electron energy of 25 keV has been measured and shows a maximum for micronuclei induction at a dose of 1 Gy. The data for 25 keV represent initial efforts to examine different portions of the LET spectrum.

Screening Mutagenized Phanaerochaete Chrysosporium for Overproduction of Organic Acids. LAURA HUBBARD (*Sacramento City College, Sacramento, CA 95822*) ROBERT A. ROMINE (*Pacific Northwest National Laboratory, Richland, WA 99352*). The production of organic acids through fungal fermentations that utilize renewable resources, such as agricultural by-products, is a matter of great interest. This is due to the large demand for these chemicals for the production of biodegradable polymers and specialty chemicals as well as a desire to reduce the dependency of US industries on petroleum based feedstocks. Malonic acid (MA), for example, is currently produced on a large scale from petroleum, but certain fungi can produce MA as a secondary metabolite. The target of this work was to select one of these fungi, *P. chrysosporium*, and improve its production of MA through classical strain improvement approaches. *P. chrysosporium* spores were exposed to UV light to induce mutations in an attempt to develop a strain that would overproduce MA. These treated spores were then divided among two thousand pH-indicating plates. The resulting colonies that showed acid production were transplanted to new plates for isolation and purification. Spores produced from these plates were used to inoculate PDA slants, and when the colonies in the slants had matured spores were harvested from them and used to inoculate shake flasks. The shake flasks were analyzed via IC to determine which organic acids were being produced and in what amount. IC data showed that the generalized mutation significantly lowered the production of oxalic acid, but had little effect on MA production. More research is needed to optimize this mutation, eliminating oxalic acid production completely so that the biosynthesis of other acids can be maximized.

Microbiology Studies On The Well Waters From DOE's South Oyster Field Research Site. NICOLE HUNTER (*Washington State University, Pullman, WA 99164*) SHU-MEI LI (*Pacific Northwest National Laboratory, Richland, WA 99352*). This project was started to test bacterial transport, which has a growing interest for its use as a viable remedial option. Oyster, Virginia was the chosen site for this project because of its shallow, unconfined sandy aquifer containing iron and aluminum oxyhydroxides, its separate zones of oxic and suboxic groundwater in close proximity and its proximity to sites that can be excavated for intact core collection and direct examination of sediment structure. The microbial flora of the Oyster site is being analyzed for changes in species diversity due to injection of foreign microbes into the surrounding sandy aquifer. Analysis of the area is an ongoing effort and the data

that has been collected is still pending on future data before it can be analyzed.

Investigation of Habitats Within the Fermi Accelerator Laboratory in Illinois That Are, and Are Not Currently Occupied by Breeding Henslow's Sparrows. MERILEE JANUSZ (*University of Illinois, Chicago, IL 60607*) PETER KASPER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The appearance of Henslow's Sparrow to the restored prairies and maintained grasslands of the Fermi Accelerator Laboratory in Batavia, Illinois is an indicator that upkeep and maintenance efforts are successful, and therefore more desirable native species may soon be appearing. This study involves the evaluation of such lands in hopes to maintain continued success. The Henslow's Sparrows were identified and counted. This bird has been found to be very particular in habitat selection. The birds have been observed in a number of varying habitats. The discovery of a loose colony of breeding Henslow's called for a comparison of unlike areas containing high populations, few species, and no species. This research compared several habitat characteristics. Transect studies were conducted to provide information regarding vegetation height, species richness, and Index of Diversity. Birds were observed to determine the likeness of territorial behavior, and to assess population numbers. Data indicates that Henslow's sparrow is indeed territorial, occupying the same perch and area of land for the migratory period. The data suggests that there is a higher population in areas with less plant diversity, and lower vegetation heights. Further research may be conducted to identify area preference according to the choices made by earliest arriving birds in future seasons.

Investigation of Sex-Determining Genes in *Populus trichocarpa*. HARVEY JONES (*Madisonville Community College, Madisonville, KY 42431*) LEE GUNTER (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Fossil fuels are becoming increasingly costly in terms of environmental and natural security issues. Scientists have been searching for environmentally friendly, renewable sources of energy to satisfy the mounting energy demand. *Populus trichocarpa* hybrids in fast-growing, short rotation woody biomass plantations can be cultivated at an accelerated rate compared with other woody vegetation, and benefit the ecosystem by returning large amounts of carbon to the soil. The sex of the poplar, a dioecious tree, is a paramount factor when considering utilizing it as a source of bio-fuel. The main objective of this research is to identify the specific sequences in the poplar genome responsible for regulating sex expression. Being able to manipulate the sex of the organism will allow measures to be taken to control reproduction and consequently increase yields of bio-fuel. The method used to find these particular genetic sequences involves identifying sequences that appear in one sex but not in the other. We are using synthetic oligonucleotide primers to amplify possible sex-linked sequences via polymerase chain reaction (PCR) to obtain information of the genes contained in male and female genotypes. If the products resulting from PCR amplification are the expected size for the target gene, further effort is applied through the process of cloning, to replicate target sequences, and gene sequencing, to verify target genes. Certain target genes have reached the sequencing stage and are in the process of being analyzed.

p21 Expression During Lens Fiber Cell Differentiation and After Radiation Damage. JAMES KIM (*Seattle Central Community College, Seattle, WA 98122*) ELEANOR BLAKELY (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The cyclin-dependent kinase inhibitor (CDKI) p21CIP1 is important to cell-cycle regulation during normal differentiation and after DNA damage. This project investigated p21 protein expression in human lens cells that differentiate from epithelial-to-fiber-type cells in vitro. Data obtained demonstrate the role of p21CIP1 in normal differentiation, and altered p21 expression after exposure to a single 4 Gy dose of X-rays. HLE cells irradiated with 4 Gy of X-rays demonstrate an induction of the p21 protein that is evident as early as 3 hours after exposure, and increased ~3 fold 12 hours after exposure. HLF cells irradiated with 4 Gy of X-rays also demonstrate an upregulation of p21 protein that is 1.6-fold at 3 hours after exposure, and is increased ~2 fold 12 hours after exposure. This data needs to be replicated, but indicate that p21 expression plays a role in the signaling mechanisms in normal lens fiber cell differentiation, and in the response of lens cells to radiation damage. Radiation-induced changes in expression of p21 may be involved in radiation-induced cataractogenesis.

The Identification of Single Nucleotide Polymorphism in Baboon Cholesteryl Ester Transfer Protein Gene for Human-Baboon Comparative Analysis. MICHAEL LAM (*University of California Berkeley, Berkeley, Ca 94720*) JAN-FANG CHENG (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The study of single nucleotide polymorphism (SNP) is a promising methodology in studying complex diseases. Our goal here is to identify the locations of SNPs in cholesteryl ester transfer protein (CETP) gene in baboon (*Papio hamadryas*) and to perform a comparative analysis with known SNPs in human CETP gene. CETP is responsible for the transfer of cholesteryl ester from high-density lipoprotein (HDL) for triglyceride in low-density lipoprotein (LDL) and very low-density lipoprotein (VLDL), and therefore influences the HDL level in plasma, which is closely associated with the risk of coronary heart disease (CHD). Twenty baboons (40 chromosomes), selected carefully from the pedigreed baboon colony supplied and maintained by the Southwest Foundation for Biomedical Research (SFBMR) and Southwest Regional Primate Research Center (SRPRC), were utilized for CETP-SNP detection. Forty-five PCR amplified products with average size of 1.5kb covered the 26.3kb CETP gene and 20kb flanking region 5' and 3' from the gene. By high-quality sequencing and assemblies, 402 SNP locations were identified and positioned in the baboon CETP region, four of which lie in the 5' and 3' untranscribed region (UTR). The average density of the SNP is 117bp, a density that is 1.4-fold higher than observed in human CETP gene. The high frequency and diversity of genetic variation detected in baboon CETP may support association studies of rare alleles in human complex diseases involving lipoprotein metabolism.

Growth and Survival of Columbia River Bivalves Partitioned by Community and Substrate Types. KYLE LARSON (*University of Idaho, Moscow, ID 83843*) BRETT TILLER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Assessing bioaccumulation of selected contaminants on the Hanford Site involves a wide variety of disciplines, interagency objectives, and species of concern. For members of PNNL's Surface Environmental Surveillance Project (SESP), studying the relationships between groundwater contamination, benthic organisms, and secondary consumers in the Columbia River along the Hanford Reach has become one of their primary concerns. In particular, the use of Columbia River bivalves as indicators of environmental stress has been focused on as a valuable tool to be used in future risk assessment and closeout processes. However, in order to compare measurable biological metrics of bivalves in sites of concern, we must be able to gather quantitative and qualitative reference data within ideal control sites and develop a field-based method for doing so. By conducting an in situ study we plan to measure typical growth and survival rates of Asiatic clams (*Corbicula fluminea*) and construct data sets that may be used in comparison in future contaminant studies. In order to properly interpret growth and survival data, we must also characterize the intrinsic variables that affect growth such as community and substrate types, primary productivity, and water conditions. We will also examine the utility of two in situ study techniques and evaluate their utility in the field as well as application for our study purposes.

The Effects of Aclarubicin on Cytochrome P450 3A. DONNA LEE (*Sacramento City College, Sacramento, CA 95822*) RICHARD ZANGAR (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Cytochrome P450 3A (CYP3A) is responsible for the metabolism of over 50% of all prescribed drugs. This broad substrate specificity leads to altered CYP3A activity during multiple-drug therapy. Understanding the mechanisms by which CYP3A catalyzes biochemical reactions is important in studying the adverse effects of drug-drug interactions. It has been reported that aclarubicin inhibits the formation of high molecular weight CYP3A (HMW CYP3A), an initial step to CYP3A degradation, by inhibiting the 26S proteasome, which is consistent with the ubiquitin/proteasome protein degradation pathway. However, initial studies have shown that proteasome inhibition actually leads to accelerated loss of CYP3A. In this study, we investigated the possibility that aclarubicin is a CYP3A substrate. Microsomes were treated with aclarubicin in the absence of proteasomes and analyzed by Western blotting to examine the formation of HMW CYP3A and to track ubiquitin. An erythromycin N-demethylase assay was conducted to examine the effects of aclarubicin on the metabolism of CYP3A substrate. We found that aclarubicin continued to inhibit the formation

of HMW CYP3A, and ubiquitination was not altered in spite of inhibited degradation. Aclarubicin also inhibited the metabolism of erythromycin, which suggests that competition between substrates may have occurred. These combined results open up the possibility that the stabilization effect of aclarubicin may be a consequence of substrate-mediation and not proteasome inhibition as previously believed. This suggests that the degradation of CYP3A may involve a new novel mechanism independent of the classical ubiquitination pathway.

Examining Processes to Fabricate a Compound Refractive X-ray Lens from Lithium. JONATHON LEUNG (*Richard J. Daley College, Chicago, IL 60652*) ALI KHOUNSARY (*Argonne National Laboratory, Argonne, IL 60439*).

There has been ongoing research to design refractive optics that can focus x-rays with the potential to significantly enhance micro-imaging techniques used today. The focusing is done by placing a number of lenses in series (a compound refractive lens or CRL) to refract an x-ray beam many times in small increments. The material of the lens affects its ability to deflect and absorb x-rays; the best lens deflects x-rays with minimal absorption. Compounds that have these properties tend to also have low Z-numbers (atomic numbers). Refractive lenses fabricated from various materials, such as aluminum, beryllium, and to some extent lithium have met with some success in focusing x-rays. Our goal is to design a manufacturing process for a CRL fabricated from lithium, a soft, malleable substance that sticks to most metal surfaces, and even to slippery surfaces such as Teflon. Despite the difficulties of working with lithium, it remains the best material for a CRL in the low to medium (2-30 keV) x-ray energy range. To design the lens, consideration is given to the physical properties of lithium, the handling of lithium and the process for fabricating the lens. The fabrication process that works best must be investigated and refined in future research. Injection molding, extrusion, pressing and stamping were considered in designing the lens. Extrusion was chosen as the first design process because of relatively low costs to manufacture components needed for this process, interchangeable die plates for single and multiple lens extrusion, no components that need to be released from lithium that could cause sticking, and previous experience in extruding an aluminum CRL.

Development of a Preliminary Physiologically Based Pharmacokinetic Model for 1,2-Diethylbenzene in F344 Rats. KERRY LEWIS (*Washington State University, Pullman, WA 99163*) KARLA D. TRHALL (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Diethylbenzene (DEB) is a colorless liquid used as an intermediate in the production of divinylbenzene, as a heat transfer fluid, and can also be found in gasoline, kerosene, and No. 2 Fuel Oil. The objectives of the current study focused on obtaining information about in vivo measurements of metabolism in the rat, and development of a preliminary PBPK model. A physiologically based pharmacokinetic model (PBPK) can be used to describe absorption, distribution, metabolism, and excretion of a compound within the body. Adult male F344 rats were used in a series of gas uptake system studies, and partition coefficients were measured using fresh rat blood. Initial 1,2-DEB exposure concentrations for gas uptake studies were approximately 750 ± 32 ppm. The blood-to-air partition coefficient determined here (175 ± 17) compared well to the previous value of 164. The metabolic rate constants, determined by the PBPK model, suggested very little DEB metabolism occurred during the exposures. By using a PBPK model, to describe the kinetics of a chemical in experimental animals, such as rats, can be used to help predict how DEB will behave in humans.

SubBase: Protein Subunit Database. RICHARD LUSK (*University of Chicago, Chicago, IL 60637*) NATALIA MALTSEV (*Argonne National Laboratory, Argonne, IL 60439*).

The subunit database is a collection of all known and hypothesized protein subunits indexed to facilitate convenient and accurate comparisons of protein composition across phylogenetic groupings. The data are drawn from all fully sequenced genomes in Swiss-Prot and TrEMBL and presently supported with annotations from the same. The dataset was expanded beyond the incomplete annotation available with a combination of loose gathering parameters and computational prediction of each possible subunit's enzymatic function and other properties necessary for sorting. This data expansion and the

integration of the complete set of completed genomes into the database allows for an elsewhere-unavailable accurate analysis of protein subunits over wide ranges of species.

Investigation of the Link Between Increased Hexose Content and Decreased Rubisco Content in Glycine Max When Exposed to Elevated CO₂. JASON MAHONEY (*Community College of Rhode Island, Warwick, RI 02889*) ALISTAIR ROGERS (*Brookhaven National Laboratory, Upton, NY 11973*).

An experimental program using free air CO₂ enrichment (FACE) has been developed to examine the effects of increasing [CO_{2,atm}] on plants and ecosystems. The FACE system allows plants to live at realistic [CO_{2,atm}] conditions expected to exist in the mid 21st century. FACE allows assessments of the effects of rising [CO_{2,atm}] on terrestrial plant life, and what impact these effects will have on the global carbon cycle. This particular investigation is an analysis of the link between carbohydrate and protein fluctuation in Glycine max (soybean) at elevated [CO_{2,atm}]. It is considered that hexokinase, in addition to being a glycolytic enzyme, acts a hexose sensor, repressing the transcription of photosynthetic genes when sensing an accumulation of carbohydrate, ultimately leading to a down-regulation of Rubisco. It is also believed that increased sucrose levels and sucrose cycling result in sink limitations, which accentuate acclimation of photosynthetic activity at elevated [CO_{2,atm}]. Ethanol soluble sugars (glucose, fructose and sucrose) were extracted from the samples and analyzed, respectively, using an enzymatic assay. Protein levels were analyzed using the SDS-PAGE and Pierce methods. After analyzing the data, it is clear that elevated levels of [CO_{2,atm}] stimulated carbohydrate production. Contrary to expectations, clear evidence of a down-regulation of Rubisco was not observed. The data suggests that current hypotheses regarding the link between carbohydrate stimulation and Rubisco down-regulation are not accurate and additional factors, such as nitrogen availability, may play a key role in the reduction of Rubisco activity at elevated [CO_{2,atm}].

Multi-dimensional Chromatography for Proteomic Analysis of *Shewanella oneidensis*. LINDSAY MAY (*University of Puget Sound, Tacoma, WA 98416*) HEATHER MOTTAZ (*Pacific Northwest National Laboratory, Richland, WA 99352*).

One of the analytical challenges of proteomics is to obtain complete protein coverage of an organism. Several approaches have been developed to meet these analytical challenges, most of which rely on the separation of peptides generated from proteome digests followed by reversed-phase liquid chromatography-tandem mass spectrometry (LC-MS/MS). To increase peptide identification, proteins were separated using size exclusion chromatography. Fractions obtained from this separation were digested with trypsin. The resulting peptides from each fraction were further partitioned using cation exchange chromatography. Finally, the cation-exchanged peptides were analyzed by LC-MS/MS. This approach was applied to the proteome of the bacterium *Shewanella oneidensis*. Using only size exclusion chromatography and LC-MS/MS, a nearly four-fold increase in the number of peptides was observed, with a concomitant three-fold increase in the number of proteins identified, when compared to only a single LC-MS/MS analysis of the entire digested whole cell lysate. Currently, size exclusion chromatography is being used on the peptides present in each size exclusion fraction. This additional chromatographic separation will lead to a pronounced enhancement in proteome coverage. This three dimensional approach provides a method for generating protein databases using a modest amount of sample obtained from various organisms and cell types.

Analysis of High Molecular Weight DNA From Human Melanoma Tissue Culture Cells After Exposure to UVA and UVB Light. SABINE MAYARD (*Queens College, Flushing, NY 11367*)

RICHARD B. SETLOW (*Brookhaven National Laboratory, Upton, NY 11973*).

Sunlight exposure is a major factor in melanoma induction in humans. But the wavelength regions are not well known characterized. There are two wavelength ranges of UV that can be absorbed by melanin containing cells; UV-A (320-400nm) and UV-B (280-320nm). It has been showed that DNA does not directly absorb UV-A but it is on the other hand a risk factor for melanoma in certain species of fish. The hypothesis being tested is that intracellular melanin exposed to UV light causes mutation via an indirect mechanism. (Setlow, R.B., unpublished communication.) This project along with others will attempt to prove or

disapprove this hypothesis. Dr. Marianne Berwick of Memorial Sloan-Kettering Cancer Center has provided us with two different cell lines of human melanoma tissue culture cells; SK-Mel 188 contains copious amounts of melanin and SK-Mel 28 contains much less melanin. The DNA of SK-Mel 188, which is more pigmented, should be affected more by UV-A exposure because the melanin in these cells absorbs UV-A, which is believed to cause mutations via the indirect mechanism activated through a melanin complex. DNA damages induced were detected by quantitative gel electrophoresis. DNA was extracted and treated with an enzyme that makes single stranded breaks next to cyclobutane pyrimidine dimers. The dimers are made by UV-B and not by UV-A exposure. The next step is to treat the DNA with an enzyme called UVrABC nuclease that will be able to make breaks at both dimers and the UV-A induced melanin related products.

The Effects of Pressure Change and Elevated Dissolved Gas on the Formation of Head Lesions in Juvenile Fall Chinook Salmon. GEORGE DARREN MAYER (*Peninsula College, Port Angeles, WA 98362*) SCOTT ABERNETHY (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Declining salmon stocks have become a major concern in the Columbia and Snake Rivers. Out-migrating juvenile salmon passing through dam turbines are exposed to conditions not encountered in free flowing river systems. Fish may be exposed to elevated gas levels due to increased spill and rapid pressure changes if they pass through turbines. The objective of this project was to produce and quantify head lesions on juvenile chinook salmon (*Oncorhynchus tshawytscha*) that were subjected to gas levels and pressure regimes that may be encountered during turbine passage. Results of this project showed that clinical symptoms appeared in 24.8% of the fish tested. These results suggest that elevated gas levels along with pressure changes similar to conditions experienced during turbine passage may have a physical affect on salmon and may be the source of cranial lesions. The relatively high frequency of cranial lesions in this project supports the need for further research to determine the effects of pressure and elevated gas exposures and to determine if there is a correlation between juvenile cranial lesions and cranial lesions in adults. If a correlation between cranial lesions in adults and juveniles and turbine passage can be made it may affect the way dams are operated or designed to make them more fish friendly.

Cryocrystallography of *Rhodobacter sphaeroides* Membrane Proteins. JOY MAYFIELD (*University of Iowa, Iowa City, IA 52242*)

PHILIP LAIBLE (*Argonne National Laboratory, Argonne, IL 60439*). Deciphering membrane protein structures is integral to rational drug design and understanding life processes. The Reaction Center (RC) and Cytochrome c_v (Cyt c_v) membrane proteins from *Rhodobacter sphaeroides* were studied. There were two different aspects of this project: crystallizing Cyt c_v, and finding a suitable cryoprotectant for RC protein crystals. It was necessary to grow the bacteria and purify the proteins before they were used in crystal screens. The Cyt c_v screens did not produce crystals, but they are useful in narrowing the protein and precipitant conditions for future trials. Trials at polyethylene glycol 4000 concentrations of 0 – 6 w/v %, 0 – 500mM NaCl, and 30 mg/ml Cyt c_v could be tested in the future. The optimum protein concentration may lie between 30 and 50 mg/ml. Many cryoprotectants were tested for "ice rings" at cryogenic temperatures. Polyglycines are not suitable cryoprotectants, but 28.6 w/v % ethylene glycol gave positive results. Ice rings were not visible in the X-ray diffraction patterns, and resolution was 3.5 – 3.6 Å. When comparing data from two RC crystals, the best method of introducing the cryoprotectant is by soaking it in an increasing gradient of ethylene glycol.

Recombinant Protein Expression of a Novel XPG Associated Protein, XAP1. COLLEEN MCCLEAN (*Fresno City College, Fresno, Ca 93611*) PRISCILLA COOPER AND JILL FUSS (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

The Diseases Xeroderma Pigmentosum and Cockayne Syndrome are rare inherited genetic disorders resulting from mutations in genes involved in DNA Repair. Both diseases arise from mutations in XPG, a gene that codes for a protein involved in enzymatic functions in Nucleotide Excision Repair, as a co-factor in global Base Excision Repair, and is required for Transcription Coupled Repair. XPG interacts with a number of other proteins involved in DNA repair. Recently two novel proteins were discovered and found to be associated with XPG

through a coimmunoprecipitation. These proteins were isolated and named XAP1 and XAP2 for XPG Associated Protein 1 and 2. XAP1 has been shown to contain two domains already known to be involved in DNA repair. This knowledge increases the likelihood that XAP1 is involved in DNA Repair. XAP1 was also found to contain a helical domain with secondary structure predictions, and a novel domain called the Repeat domain. This domain contains a 41 amino acid sequence that repeats 18 times and is conserved in mouse, rat, cow, and human XAP1 proteins, indicating its importance. In order to perform crystallographic and antibody studies on XAP1 it is necessary to express each of the domains as protein. To do this the gene sequence of XAP1 was divided into 5 domains, each of which was subcloned into two commercially obtained vectors tagged with different antibody markers. Each of these plasmids was then transformed into three expression strains and expressed to determine the best time and temperature of protein expression.

Scanning for ENU-Induced Mutations in the Mouse *Herc2* Gene. JEREMY MCDUFFIE (University of Tennessee at Knoxville, Knoxville, TN 37849) MITCHELL KLEBING (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The *Herc2* gene is located in the juvenile development and fertility-2 (*jd2*) locus of mouse chromosome 7. Eleven N-ethyl-N-nitrosourea (ENU) mutations have been found to produce the *jd2* phenotype, which is characterized by runting, jerky movements, male sterility, and shortened life span. Previous studies of three of these mutations showed that they are located in the *Herc2* gene. The remaining *jd2* ENU mutations are expected to also be mutations in the *Herc2* gene. Therefore, this study is aimed at identifying these ENU mutations. To do this, RT-PCR experiments are being performed in order to look for size alterations in products of the mutant mice, which when found will be sequenced to determine the effect the alteration has on the encoded protein. In the second phase of this study, mutations in which no size alteration is observed will then be studied for the presence of single nucleotide substitutions in RT-PCR products using hetero-duplex analysis. Further progress will be reported as sufficient data becomes available.

Drug Addiction Research and "Online Classroom" at Brookhaven National Laboratory. BARBARA MELENDEZ (University of Puerto Rico, Cayey, PR 00782) BRIAN MURFIN (Brookhaven National Laboratory, Upton, NY 11973).

The goal of this project is to create awareness of the damage that drugs can cause, and other problems associated with drug addiction. Research involving dopamine and drug addiction was observed in the Chemistry Department. Using the information obtained, an educational module was created. Inquiry based learning activities will help students understand the effect of drugs on the brain. The module was converted into web pages and will be tested by high school students. This is a work in progress that will be continued by the Brookhaven National Laboratory "Online Classroom" team.

Rapid Compositional Analysis of 61 *Zea mays* Samples Using Near-infrared Spectroscopy. JONATHAN MEUSER (University of California, Davis, CA 95616) STEVEN THOMAS (National Renewable Energy Laboratory, Golden, CO 89401).

A major challenge in commercializing ethanol production from corn stover is the great variability in composition of commonly grown varieties. Only when the variables that determine stover composition are isolated can optimum stover be produced, making possible consistent process yields and economics. The extent to which environmental and genetic factors affect cell wall composition in corn stover is unknown. In this study, the cell-wall composition of 61 stover samples was determined by near-infrared spectroscopy (NIR). With NIR, the composition of many samples can be economically, accurately and quickly determined, providing the bulk of data necessary to perform meaningful statistics. As we approach a high-throughput system of compositional analysis, outlying samples and the variables that cause their dissimilarity may be more readily understood. For instance, though closely related to commercial corn, *Teosinte parviglumis* drastically differed in composition. Also, Pioneer B73xMo17 and Pioneer 33P67 were tested to determine the affect of irrigation, planting density and variety on cell-wall composition. These variables proved to be insignificant factors in composition, however, 33P67 grown under the same conditions had unusual variability in soluble sugars. Because irrigation and planting density commonly differs between fields, eliminating these two variables as factors affecting

composition allows greater flexibility in growing and experimenting on high value stover. Further research into the exact cause of *Teosinte's* structural differences may illuminate genetic causes of cell-wall variation for all corn.

Leaf Area Measurements and Water Relationships of Juvenile and Mature (*Artemisia tridentata*) Big Sagebrush at the Hanford Site. BENJAMIN MILES (Grambling State University, Grambling, LA 71245) FENTON KHAN (Pacific Northwest National Laboratory, Richland, WA 99352).

A study was conducted during the summer of 2002 to examine the leaf area to biomass of juvenile and mature (*Artemisia tridentata*) big sagebrush shrubs. Because *A. tridentata* is a dominant native shrub species on the Hanford Site, estimates of water use are needed to aid in calculating recharge rates for a proposed Immobilized Low-Activity Waste (ILAW) Disposal site. It is hypothesized that there is a 1:1 correlation between the leaf area to biomass ratio between juvenile and mature sagebrush at a proposed ILAW disposal site. This investigation will contribute to ongoing studies of water use estimates of sagebrush shrubs at proposed disposal sites on the Hanford Site. Although additional studies are needed, composite data from 99 and Summer 02 suggest a 1:1 correlation ratio of leaf area to biomass does not exist between juvenile and mature big sagebrush because mature shrubs appear to have a greater leaf area to biomass.

Differential Expression Analysis of Subtelomeric Genes in Mice with Telomere Dysfunctions. MARSHALL MILLER (Appalachian State University, Boone, NC 28608) YIE LIU (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Telomeres, the repeated code that marks the end of chromosomes, have been linked to both aging and cancer. In mammals the sequence TTAGGG is repeated forming a long strand that, held together with telomere binding proteins, forms a unique structure known as a T-loop. Normally telomeres affect adjacent genes in the subtelomeric region by suppressing their expression. This effect has been described in yeast and mammals as Telomeric Position Effect, or TPE. Telomere dysfunction would, on the other hand, cause a loss of TPE and alter the expression of some genes on the subtelomeric region. To study this, a search for mouse subtelomeric genes will be conducted first, followed by an examination of their expression on animals with normal or short telomeres using Northern blot and micro-array techniques. This will then be followed up by a nanotechnological survey in order to study differential expression throughout the whole mouse genome. To search for the expressed sequences or genes on the subtelomeric region, the first mega-base of the NCBI, ENSEMBLE, and UCSC mouse databases were searched and logged. This log was then BLASTed against the NIA mouse 15k cDNA clone library. About a quarter of the genes identified as being in the subtelomeric region were found in the mouse 15k. These will be obtained from NIA, the rest will be ordered from commercial distributors. These clones will be used for the differential expression analysis on mice with long and short telomeres. Results of these studies will be presented.

Site-Directed Mutagenesis in Calmodulin and its Applications. KARAM MOON (University of Washington, Seattle, WA 98105) THOMAS SQUIER (Pacific Northwest National Laboratory, Richland, WA 99352).

The use of genetically-encoded affinity tags is a commonly used standard method of purifying and studying proteins. While most tags are small-molecule binding proteins, the size of these proteins can have potential alteration effects on the activity of the protein to which they are fused. Less perturbing are a few short peptides, such as a recently developed fluorescent dye that specifically interacts with tetracycline containing helices, known as FIAsH (Fluorescein Arsenical Helix binder). (Thorn, 213) FIAsH has been shown to bind with proteins modified with a CCXXCC containing helix. Polymerase Chain Reaction (PCR) has emerged as a powerful and precise in vitro method for altering a particular template sequence by introducing new sequence information adjacent to the target by use of primers to create site-directed mutations. (Burke, 1) In particular, modifying the N-terminal peptide sequence of chicken CaM to contain the sequence CCXXCC will allow for future applications and studies, using the FIAsH tag. In the present study, overlap PCR techniques have been utilized to create this site-directed mutation, so that the CaM can be expressed in a prokaryotic system, and recombinant CaM can be purified using a bis-arsenic fluorescein. In addition, these studies are directly appli-

cable to the goal of expressing and characterizing protein complexes for the Genomes to Life (GTL) initiative, funded by the DOE.

Curating a Database of Functional RNAs in E. coli for Use in a Novel RNA Gene-finding Algorithm. DENTON MUNNS (Southern Utah University, Cedar City, UT 84720) STEPHEN R. HOLBROOK (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The bacterium *Escherichia coli* is the best characterized organism known and serves as the model for development of computational methods aimed at understanding cellular functions. In addition to messenger RNA that encodes proteins, DNA also encodes functional RNA molecules. These functional RNAs, or fRNAs, are also known as ncRNAs, or non-coding RNAs. Recently, methods have been developed for the identification of fRNA genes in genomic DNA. Our studies have been twofold: 1) Creation of a MySQL database of 162 reported and experimentally verified, fRNAs in *E. coli*, including reference, function, sequence, operon structure, predicted secondary structure and location of homologues in other organisms; and 2) application of these sequences for parameterized training of Support Vector Machines to learn to identify other novel fRNAs in the *E. coli* genome.

Modulation of Integrin Expression During Lens Fiber Cell Differentiation and After Radiation Damage. RACHEL MUSTAIN (Merced College, Merced, CA 95348) ELEANOR BLAKELY (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Integrins are cell adhesion molecules (CAMs) that play an essential role in anchoring cells to the extracellular matrix. We have preliminary evidence showing that proton irradiation moderates b1-integrin expression in Human Lens Epithelial cells (HLE) and Human Lens Fiber cells (HLF) with a shift in intracellular distribution. In the present study, we compared levels of alpha-6A, alpha-6B, and β 1 integrins in total protein extracts from X-ray irradiated and non-irradiated HLE and HLF cells using gel electrophoresis and Western analysis. Cells were grown on bovine corneal endothelial-derived ECM in media containing 15% fetal bovine serum and 5 ng/ml FGF-2. Proteins were harvested from both epithelial and fiber cells at four different stages of growth: Days 3, 12, 19, and 25. Single doses of 4 Gy X-ray (150 kVp) were given to cultures and the total proteins were harvested in a time course after exposure from 0.5 to 12 hrs. Western Analysis was completed using the NuPage electrophoresis system. Antibodies for these studies were obtained from Transduction Labs (mouse monoclonal b1 integrin) and from Santa Cruz Biotech (goat polyclonal a6 integrins). The results indicate that the cultured human lens model demonstrates the a6 isoform switching reported during differentiation from epithelial to fiber cells in vivo. Transient changes in b1 integrin and a6 integrins were observed, primarily in the HLF cells. These radiation-induced transient changes in integrins may be important to mechanisms of radiation damage leading to cataract.

Apoptosis Induction in Human Neural Stem Cells. DAPHNEY MYRTIL (Stony Brook, Stony Brook, NY 11794) MARCELO VAZQUEZ (Brookhaven National Laboratory, Upton, NY 11973).

During long-term space missions, a significant fraction of the neurons and other cells in an astronaut's brain would be traversed by HZE particles. It has been estimated that over the course of a three-year mission to Mars, 46% of brain neural cells will be subject to a direct hit by a HZE particle ($z > 15$), with 13% of the neurons traversed by a Fe ion. This clearly demands that we define the damage, which may be incurred by heavy ion exposure. There are at least two mechanisms by which neural stem cells and neurons can die, apoptosis and necrosis in that the former generally is considered to be an active process requiring synthesis of particular proteins responsible for cell killing. Furthermore, internucleosomal cleavage of DNA and nuclear fragmentation often accompany apoptosis whereas cellular swelling, membrane disruption, and random cleavage of the DNA typically accompany necrosis. Many insults, including low-LET radiation appears to induce stem cells and neuronal death via apoptosis both in vitro and in vivo models. Nevertheless, the molecular and cellular changes responsible for radiation-inducing neuronal apoptosis are unknown. In the present study we measured the expression of apoptotic markers induced by radiation and serum deprivation in neuronal precursor cells (NT2, STRATAGENE) as a model for adult neural stem cell system.

Attempts at Protein Crystallization of *Vibrio cholerae* 1652 and *Pseudomonas aeruginosa* 3947. CALLIE NAGY (Washington State University, Pullman, WA 99164) NANCY ISERN (Pacific Northwest National Laboratory, Richland, WA 99352).

Bacterial microbes can form into complex films (biofilms) that resist eradication by conventional antibiotics. Biofilms are believed to be involved in the pathogenesis of periodontal disease, prostrate infections, kidney stones, tuberculosis and Legionnaire's disease (Costerton, 2001). Structures of the proteins comprising bacterial biofilms can lend insight into the characteristics and specific functions of these proteins. Scientists may then be able to develop drugs able to interfere with the formation of biofilms and thus successfully to combat various resistant infections, such as cholera. The majority of this research project focused on the bacteria, *Pseudomonas aeruginosa* (PA), responsible for diseases in Cystic Fibrosis patients, and *Vibrio cholerae* (VC), a bacterium causing cholera. VC 1652 and PA 3947 are important genes involved in signaling within the biofilms. Determining the structure of proteins from these specific genes was the object of this research. To obtain crystals suitable for structural analysis, the genes must first be cloned and the proteins purified. The desired gene is first cloned into *E. coli* cells, which are induced to express the target protein. Then the cells are lysed, using a French press, to harvest the proteins for purification. The purified protein is run through crystallization screening to determine the best crystallization conditions. Protein structures are then obtained through x-ray diffraction. Attempts to crystallize VC 1652 are currently in the crystallization stage. The crystallization of PA 3947 has so far proved to be unsuccessful.

Preliminary Characterization of the Riparian Zone Along the Hanford Reach. ALEXANDRA NAPIER (Washington State University, Pullman, WA 99163) JANELLE DOWNS (Pacific Northwest National Laboratory, Richland, WA 99352).

Preliminary sampling and mapping surveys of the riparian plant communities along the Hanford Reach were conducted in the summer of 2002. The plant species composition, percent visual cover, frequency of species, and density of different plant functional groups in the riparian plant communities were found using a variety of environmental monitoring techniques. These methods included transects, belt transects, and species lists. Data was organized by community type. In total 16 transects were evaluated in six different community types. Community types were compared by relative percent cover of vegetative total, by relative vegetative cover by life form, and by total vegetative cover by community type. Native and introduced species totals were also compared. It was found that the *Agropyron dasytachyum* var. *smithii* and *Sporobolus cryptandrus* community types had the highest levels of vegetative cover; these communities were at elevations high enough to avoid frequent inundations, unlike the *Cyperus aristatus*, *Phalaris arundinacea*, and Non-Persistent Emergent Wetland communities. The drier *Agropyron dasytachyum* var. *smithii* and *Sporobolus cryptandrus* communities were also the only two communities with a noticeable amount of microbiotic crust, consisting of 17% and 18% total cover. The *Phalaris arundinacea* community had the highest ratio of native to introduced species, followed closely by the Non-Persistent Emergent Wetland communities. The large amounts of native species found in these areas consist mainly of native perennial grasses, 17% and 60% respectively.

Evaluation of the Genetic and Nutritional Control of Obesity and Type 2 Diabetes in a Novel Mouse Model on Chromosome 7: An Insight into Insulin Signaling and Glucose Homeostasis.

SARAH NELSON (University of North Carolina at Greensboro, Greensboro, NC 27413) MADHU DHAR (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Obesity is the main cause of type 2 diabetes, accounting for 90-95% of all diabetes cases in the US. Human obesity is a complex trait and can be studied using appropriate mouse models. A novel polygenic mouse model for studying the genetic and environmental contributions to and the physiological ramifications of obesity and related phenotypes is found in specific lines of mice bred and maintained at Oak Ridge National Laboratory. Heterozygous mice with a maternally inherited copy of two radiation-induced deletions in the p region of mouse chromosome 7, p23DFioD and p30Pub, have significantly greater body fat and show hyperinsulinemia compared to the wild-type. A single gene, *Atp10c*, maps to this critical region and codes for a

putative aminophospholipid translocase. Biochemical and molecular studies were initiated to gain insight into obesity and glucose homeostasis in these animals and to study the biological role of Atp10c in creating these phenotypes. Glucose and insulin tolerance tests were standardized for the heterozygous p23DFioD and control mice on a custom-made diet containing 20% protein, 70% carbohydrate, and 10% fat (kcal). Atp10c expression profiles were also generated using Reverse-Transcriptase Polymerase Chain Reaction (RT-PCR). Heterozygous p23DFioD animals showed insulin resistance after receiving a dose of Illetin R insulin. RT-PCR data also shows differences in Atp10c expression in the mutants versus control mice. Using these standardized biochemical assays, future studies will further the understanding of genetic and nutritional controls of glucose homeostasis and obesity in animal models and subsequently in human populations.

Design, Construction, and Implementation of New Vectors for Expression of Foreign Membrane Proteins in *Rhodobacter*.

KATIE OLSON (University of Idaho, Moscow, ID 83843) DEBBIE K. HANSON (Argonne National Laboratory, Argonne, IL 60439).

In order to study membrane proteins it is important to have an efficient method to express and purify them. At the present time the lab is using its own modified expression vector with a c-terminal jistidine tag built in. This has worked for some proteins but we would like a vector with an n-terminal histidine tag as well. Another helpful addition to the vector is a protease site to cleave off the tag after purification. The construction of these vectors required taking pieces from previously existing vectors and ordering newly designed oligonucleotides (oligos) as well. Four proteins were all successfully inserted into the new vector using NheI and BglII restriction sites but we are yet to have results that the proteins were properly expressed with the histidine tail.

Inhomogeneous Ion Channel Dynamics of Gramicidin. *DAVID PANTHER (George Fox University, Newberg, OR 97132) H. PETER LU (Pacific Northwest National Laboratory, Richland, WA 99352).*

Gramicidin has been studied for many years and is an important molecule that provides the foundation for much of what we know about ion channels. This work focuses on the study of the multi-state dynamics in the gramicidin ion channel. Patch clamping on artificially formed bi-layer membranes incorporated with gramicidin was used to record single channel current data. The current trajectories were subsequently analyzed with autocorrelation methods previously applied to single molecule fluorescence recordings. We observed that a rate fluctuating, dynamic disordered behavior generally exists for single gramicidin channel ion current trajectories. We attribute the complex dynamics to different association and dissociation states of the dimer-forming channel.

Electroosmotically Induced Hydraulic Pumping on Microchips.

CHAD PITRE (Southern University, New Orleans, La. 70126) J. MICHAEL RAMSEY (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

A common method for moving fluids through the channels of microfluidic devices is electroosmotic flow. Under the proper conditions, electroosmotic flow can also be used to pump fluids hydraulically through these same devices. The method investigated in this study was to selectively coat the microfluidic channels with negatively and positively charged polyelectrolytes to produce electroosmotic flow in opposing directions. On a microchip with a cross intersection, an electrical potential is applied across one channel coated with a polycation and one channel coated with a polyanion. Depending on the polarity of the electrical potential, the electroosmotic flow moves toward or away from the intersection creating a positive or negative pressure, respectively, at the intersection. This hydraulic pressure results in pressure driven flow in all four channels of the microchip. Initial experiments investigated the stability and electroosmotic mobility of the polyanion and polycation layers compared to a native glass surface. Microchips were coated with polyelectrolytes and the mobility determined using a buffer doped with dye and laser-induced fluorescence detection. For the hydraulic pumping experiments, the microchip was coated with the polycation, and subsequently, two of the four channels were coated with the polyanion. With the potential applied across one positively and one negatively coated channel, an average flow velocity of 0.38 mm/s was determined in one of the field-free channels with 2 kV applied.

Molecular Recognition on the Surface of Bacterial Cells Using Atomic Force Microscopy. *SAMUEL PORTER (University of Tennessee, Knoxville, TN 37916) MITCHEL DOKTYCZ (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

The atomic force microscope operates by scanning a microcantilever over a surface and monitoring the position of the cantilever in response to changes in surface topography. The instrument is sensitive enough to generate images of biomolecules such as proteins and DNA in addition to well-defined cell surfaces. Besides being capable of generating images at the nanometer level, another advantage of atomic force microscopy is the fact that this technique can be utilized in aqueous environments. We successfully generated high-resolution images of *Escherichia coli* in both dry and aqueous environments. Water, phosphate buffered saline, saline, and Luria broth were all examined according to the quality of images produced in these mediums. We were then able to combine dynamic force microscopy and simultaneous molecular recognition with the ultimate goal of localizing protein-binding sites on the surface of *E. coli* cells. In preliminary experiments, we determined the interaction forces between the ligand-receptor combination of biotin and avidin. Derivatizing microcantilevers with molecular recognition agents will allow us to identify the precise location of specific receptors on cell surfaces.

Fluorescence Measurements of Promoter-Green Fluorescent Protein Constructs. *KATHY QUACH (Sacramento City College, Sacramento, CA 95822) MARGARET ROMINE (Pacific Northwest National Laboratory, Richland, WA 99352).*

Bioremediation at the Department of Energy (DOE) sites has been a concern for many years. *Shewanella oneidensis*, a dissimilatory metal reducing bacteria (DMRB) is able to respire various metals and radionuclides at a remarkable rate and may potentially be an answer to this very complicated problem. A primary objective of this research is to understand at the cellular level how this bacterium reduces certain iron oxides. Approximately 52 various promoter-GFP constructs of *S. oneidensis* were tested to identify which promoters are expressed under different growth conditions. The goal of this short-term project was to evaluate the effects of growing cells in suspension versus on solid surfaces. Our results suggest that agar surfaces induce expression of four different promoters; two upstream to cell-cell signaling molecules, one to curli pili production, and the fourth to a pair of putative c-type cytochromes. Further tests may be conducted on *Shewanella* to determine whether AI2, a molecule that is secreted by *Shewanella* promotes communication between cells, effects expression of these promoters, and whether growth on agar surfaces induces promoters upstream to genes involved in biofilm formation. Results from these studies will help determine which constructs should be used for subsequent environmentally controlled studies in biofilm reactors and chemostats.

Homophila: Human Disease to *Drosophila* Gene Expression in Gateway. *MARTHA RODRIGUEZ (Fresno City College, Fresno, CA 93741) MARK STAPLETON (Lawrence Berkeley National Laboratory, Berkley, CA 94720).*

A ten-day life cycle and plentiful progeny has made *Drosophila* a model organism from which to study human diseases, sixty percent of which have a counterpart in the fly. To this effect, the Homophila database of 714 human disease genes and their *Drosophila* counterparts (548 genes) was used to search for 24 human disease genes that have similar genetic sequences to the clones already contained in the *Drosophila* Gene Collection of the Berkeley *Drosophila* Genome Project. The specific *Drosophila* clones containing the human homologs were prepared and inserted into a pENTR vector to create an entry clone for use in the Gateway Cloning System, a tool used to facilitate cloning of PCR products, analysis of gene function, and protein expression. The entry clone created was end-sequenced to check for insertions, deletions, or other mutations that may have occurred in the amplification process. Once sequenced-verified, this entry clone may now be used in several ways. For example, it may be used to generate an expression construct by performing a recombination reaction between the entry clone and different Gateway destination vectors. The constructs then may be used to conduct protein studies utilizing bacterial, mammalian, yeast, or insect expression systems.

Affinity Evolution of scFv Antibodies Through *Saccharomyces cerevisiae* Surface Display. PAMELA RODRIGUEZ (Northern New Mexico Community College, Espanola, NM 87532) JAMES R. COLEMAN (Pacific Northwest National Laboratory, Richland, WA 99352).

Abstract Antibodies play a major role in cancer research. A library of scFv antibodies was created for display on the surface of yeast. Single chain antibodies are a small fragment of the entire antibody that contains the antigen-binding pocket. A clone was isolated that binds a peptide of the p53 protein. Joint technologies effectively screen diverse single chain (scFv) antibody libraries and identify scFv with specific binding affinities. A mutated library was created from this scFv clone through mutagenic PCR and an individual clone with higher affinity was isolated. Affinities (Kd) were determined and compared with the parental strain (Kd = 1mM). Immuno-staining was coupled with flow cytometry to obtain their binding affinity, Kd values of individual clones and was compared with the parental yeast strain. When compared with the parental strain there were several high affinity binding mutant yeast strains found. With the completion of the human genome project and the wealth of data being generated by proteome wide yeast two hybrid analysis, knock out mice, and other studies, the need for protein specific affinity reagents become increasingly sought after. {Feldhaus, M.J., Siegel, R., et al., 2002} Affinity reagents that bind with high affinity and specificity are critical in proteomics research endeavors. Further more, these reagents are becoming essential to more deeply interrogate the functions of gene products and their relationships in disease and cellular function. {Feldhaus, M.J., Seigal, R. et al. 2002}

Microbial Community Analysis of Aquatic Sediment Cores.

LORAIN SALAS (Austin Community College, Austin, TX 78757) TAMAS TOROK (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

DNA isolation, and terminal restriction fragments length polymorphism (T-RFLP), were used to compare and analyze the microbial community diversity in core sediment samples from Lake Baikal. As part of a larger ongoing project two sediment samples from different depths were screened using the DNA isolation methods and T-RFLP. The FastDNA[®] SPIN kit for DNA isolation was deemed the best for quickly extracting community DNA from sediment samples without the undesirable chemicals used in the classical chloroform/ phenol extraction. A mixture of 16S rRNA coding sequences were amplified from community genomic DNA using polymerase chain reaction (PCR) in which one of the two primers used was fluorescently tagged at the 5' end. Restriction enzymes digested the amplified 16S rRNA allowing the analysis of fluorescently labeled fragments. Analysis was performed using an automated DNA sequencer and the GeneScan software. T-RFLP data were obtained for two sediment samples, but with minimal numbers of genetically distinct bacteria. The reasons for the poor T-RFLP data are unknown, but may be related to the need to carefully develop consistent PCR and digestion protocols for the small amounts of extracted genomic DNA.

Microbial Analysis of SDA Extraction Wells. JENNIFER SAYER (Idaho State University, Pocatello, ID 83209) BRADY LEE (Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID 83415).

Microbes enriched from vapor extraction wells located at the RWMC were cultivated and used in an experiment to determine if the microorganisms could degrade carbon tetrachloride. In previous microcosm experiments, the culture was able to reductively dechlorinate carbon tetrachloride when Fe (III) EDTA and crushed basalt were used as sources of ferric iron for respiration. The purpose of the study reported here was to determine changes in the microbial population from the microcosm experiments, and to potentially identify the species having the capability to dechlorinate carbon tetrachloride. This study was conducted by taking frozen samples from the microcosm experiments, extracting the DNA from the cells, and characterizing the DNA using various molecular techniques.

Comparing the Migration Rates of Subyearling Fall Chinook Salmon in the Columbia River During High and Low Flow Years. ADAM SEALOCK (Washington State University, Pullman, WA 99164) GEOFFREY MCMICHAEL (Pacific Northwest National Laboratory, Richland, WA 99352).

There is currently a debate among fisheries experts in the Pacific

Northwest concerning the effects of river flow on juvenile anadromous salmonid migration. An opportunity to examine the relationship between river flow and the migration rate of juvenile fall chinook salmon, *Oncorhynchus tshawytscha* presented itself in conjunction with a larger project in which a unique contrast in river flow occurred. In 2001 and 2002 hatchery subyearling fall chinook salmon were tagged with passive integrated transponders or PIT tags. PIT-tagged fish were later released in the forebay and tailrace areas of Priest Rapids and Wanapum dams on the Columbia River between June 5 and June 22 of 2001 (a low-flow year) and 2002 (a high-flow year). Migration information was obtained to McNary, John Day, and Bonneville dams. This research concludes that hatchery subyearling fall chinook salmon migrated from Priest Rapids and Wanapum dams to Bonneville Dam faster during a high-flow year. The basis for this conclusion is rooted in three key findings. First, the average migration rate of the release groups in 2002 was higher and significantly different from those of 2001. Second, in all but one comparison (11/12), it was found that the slowest fish of the high-flow year, 2002, migrated faster than the slowest fish of the low-flow year, 2001. Finally, all comparisons showed that the fastest fish in the high-flow year 2002 migrated faster than the fastest fish of the low-flow year 2001.

Habitat and Population Densities of Asiatic Clams (*Corbicula fluminea*) in Association with Growth and Survival in the Hanford Reach, Columbia River. ROCHELLE SHIPLEY (Eastern Washington University, Cheney, WA 99004) BRETT TILLER (Pacific Northwest National Laboratory, Richland, WA 99352).

There are several known contaminant seeps along the Hanford Reach of the Columbia River due to improper disposal of pollutants during the Plutonium production years at the Hanford Site. Select contaminants now exceed Washington State's ground water standards near the Columbia River. The abundantly populated Asiatic clam (*C. fluminea*) has been chosen as a biological indicator to examine contaminant uptake and assess subsequent biological impacts from the Hanford Site contaminants. These filter feeders siphon large amounts of water, phytoplankton, and sediment daily, where they accumulate pollutants. Our projects goals were to construct methods for field based monitoring of growth and survival, along with attaining the natural demographics of *C. fluminea* in the Hanford Reach. Enumerating the densities of Asiatic clams and characterizing their shoreline habitat in uncontaminated areas will be baseline data accomplished through Behr Turner's Master's thesis. The monitoring techniques of growth and survival are provided by the work of Kyle Larson. Together the two projects will provide basic comparison data and field techniques for future site assessments of biological impacts.

Determining the Activation of EGF Receptors Depending on the Availability of the Ligand. MELISSA SILVA (Western Washington University, Bellingham, WA 98225) LEE OPRESKO (Pacific Northwest National Laboratory, Richland, WA 99352).

In trying to determine what and how the cells are communicating with each other we must be able to track the ligands. Ligands and receptors are the communication network between cells. The ligands can be membrane bound or they can be released. This poses another question. How much ligand does a cell release, and how fast does it release it? By creating different chimeras of autocrine and paracrine CHO cells, we are able to see how the different cytoplasmic tails affect the pathways of the ligand release. Once we have a better understanding of this, it may be possible to prevent cell damage.

Interpreting the Novel: An XPG-related Protein's Response to Radiation. KYRSTEN STOOPS (Whitman College, Walla Walla, WA 99362) PRISCILLA COOPER (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

XAP1 is a novel protein, discovered in a coimmunoprecipitation with XPG. Due to the important role of XPG in TCR and other DNA repair mechanisms, determining the relationship of XAP1 with XPG and XAP1's biological role are important in furthering the understanding of DNA repair. WI 38 VA13 cell lines were cultured in 150 mm dishes and separately exposed to 2 Gy IR and 5 J/m² UVA radiation. Incubation points were set and cells were cultured at 37°C. Total RNA was extracted and 1.4 micrograms (IR study) and 0.8 micrograms (UV study) were reverse transcribed into cDNA. Five microliters of the cDNA product underwent PCR for 32 cycles. A preliminary study on IR exposure with real-time PCR (250 ng RNA) showed a decrease of the

mRNA of XAP1 one-hour post exposure. This result was confirmed with PCR, with a decrease in XAP1 mRNA levels starting post exposure. Ultra violet radiation did not alter XAP1 mRNA levels. Preliminary research has found correlating studies determining a decreased expression of cell cycle progression genes with ionizing irradiation (but its uncertain whether this downregulation is due to transcriptional repression or another mechanism), and another gene involved in TCR, BRCA1, showing a decrease in mRNA levels with UV exposure. These studies must be considered, and further research should be done to determine the rate, time, and mechanism (decreased transcription or increased degradation) of IR downregulation of XAP1 mRNA.

Protein Crystallization for Transmission Electron Microscopy. JULIE TAKACS (Franklin and Marshall College, Lancaster, PA 17604) BARBARA PANESSA-WARREN (Brookhaven National Laboratory, Upton, NY 11973).

To understand the function of a protein molecule the molecular structure must be determined. Traditionally x-ray crystallography has been the primary method of structure determination of three-dimensional protein crystals, but analysis with transmission electron microscopy (TEM) and electron diffraction has become a method for quantitatively examining two-dimensional (2D) protein crystals. This investigation examines various methods and conditions to obtain quality protein crystals for TEM analysis. K⁺ channel protein and photosynthetic reaction center protein were crystallized using the 'hockey stick'-dialysis tubing method and imaged. Twelve crystallizations of purified Na⁺,K⁺-ATPase using variations of the hanging drop (HD) method were analyzed and imaged with TEM. Crystallization of gC1q receptor protein was attempted with a modified HD method, and with multi-walled nanotubes. Analysis of the diffraction pattern obtained from the photosynthetic reaction center protein indicated that the crystal was not a high quality protein crystal. The Na⁺, K⁺ ATPase vesicles were imaged and showed the first stages of crystallization. The results suggest that the HD technique is more efficient at forming 2D crystals when small volumes of proteins are required for TEM. Initial imaging of the gC1qR crystals did not reveal any high quality crystals. While the hockey stick method did produce crystals, it was difficult to handle, took months to crystallize, the crystals were of poor quality, and tended to precipitate rather than crystallize. Further experimentation with the HD method may lead to more predictable crystallizations with small volumes of purified protein.

Studying the Cytochrome b5 Reductase-Cytochrome b5 Mechanism: Protein Crystallography Using Mutations in R91 and S127. DAVID TAORMINA (Stony Brook University, Stony Brook, NY 11794) MARIA BEWLEY (Brookhaven National Laboratory, Upton, NY 11973).

Electron transport via cytochrome b5 reductase and cytochrome b5 is a key mechanism used by the cell to drive its metabolic and physical processes. At the core of this system is the transfer of electrons from NADH to FAD. The FAD binding site has been well characterized in the literature and has a highly conserved flavin-binding motif RXY(T/S)+(T/S). The phosphate moiety is housed in a positively charged environment due largely to the side chain of R91. Previously, a number of R91 point variants were shown to exhibit altered flavin circular dichroism and kinetic properties, including altered substrate binding. Surprisingly, characterization of a methemoglobinemia-causing mutant, S127P, behaved with similar characteristics. In order to understand the nature of the observed spectral changes, and gain further insight into the disease-causing mutant, we have embarked upon crystallization studies that will be followed up with the structure determination by others in the group.

Homophila: Human Disease to Drosophila Gene Expression in Gateway. TAMARA THORESON-OROZCO (California State University, Fresno, Fresno, CA 93740) MARK STAPLETON (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The study of *Drosophila melanogaster* has played a very important role in genetics research. A large percentage of human disease genes that have been discovered so far closely resemble genes found in *Drosophila*. Due to this fact, *Drosophila* can be used as a model organism to study the functions of human disease genes. The purpose of the research conducted was based on whether human diseases can be studied using related genes found in *Drosophila*. The goal was to create an entry clone using a universal cloning system called

Gateway. Gateway facilitates the study of genes by easily cloning and moving them into expression systems. The Homophila database at UCSD was used to identify potential disease genes found in *Drosophila*. Once the complete sequence of the related gene was identified, forward and reverse primers were designed to perform polymerase chain reactions (PCR). PCR reactions amplify the open reading frames, and through various methods, place them into the Gateway cloning system as an entry clone. Creating the entry clone was a successful part of the research being conducted. If time had permitted, the entry clone would have been transferred into multiple destination vectors. Once in multiple destination vectors, the gene becomes an expression clone from which different types of living cells can express the gene as protein. Protein expression is important in studying the structure and function of genes in humans and *Drosophila*. Techniques such as the Gateway system will also benefit other genome projects in the future.

The Effects of Intertidal Elevation and Transplantation on the Morphology and Productivity of Eelgrass (*Zostera marina*) in Sequim Bay, Washington. FRANCES VAN CLEVE (Smith College, Northampton, MA 01063) RON THOM (Pacific Northwest National Laboratory, Richland, WA 99352).

Eelgrass shoot density, daily shoot growth rates, and net productivity were measured to determine the effect of elevation on morphology of leaves over two-week periods during summer 2002. Four sites spanning the intertidal distribution of eelgrass were established. Plants were counted and marked with a needle, and leaf width and length were measured. Transplants were exchanged between two of the elevations to assess eelgrass' ability to adapt to changes in light; photosynthetically active radiation (PAR) was measured at all four elevations. Shoot density was highest at mid-elevations (-0.2 ft relative to mean lower low water) and decreased with depth. Shoot growth rates were highest at the lower elevations (-1.7 ft), followed by mid-elevations. Net productivity was high at both the lowest and mid-elevation sites. After two weeks, eelgrass transplanted from low to mid-elevations increased leaf area, daily shoot growth, and net productivity compared with controls, whereas transplants from mid to low-elevations decreased shoot density, leaf area, daily shoot growth, and net productivity. These changes are likely a result of adaptations to different elevations and associated environmental stressors. For example, at shallow sites, desiccation can limit eelgrass growth, whereas at deep sites, availability of light is a limitation. Thus, eelgrass adapts to shallow sites with high shoot density and small leaf area; deeper sites are characterized by low densities and larger leaf areas. The results presented in this study provide information about eelgrass biology, which could be used in restoration efforts and as a basis for further investigations.

The Purification of Adenovirus Protease Serotype 2. MITEN VASA (Cornell University, Ithaca, NY 14853) WALTER F. MANGEL (Brookhaven National Laboratory, Upton, NY 11973).

Virus-coded proteases are one of the most attractive targets for anti-viral agents. Many RNA and DNA viruses require proteases for the synthesis of infectious virus. Therefore, it is essential that this enzyme be produced in large amounts and purified for experiments that could lead to anti-viral agents. For making large amounts of enzyme, modern molecular and biochemical methods involve exponential growth of bacteria transformed with vectors that, once induced, continuously transcribe a gene that was ligated into the vector using restriction enzymes. The vector is constructed to also transcribe genes for antibiotic resistance in order to be able to select only for bacteria transformed with the vector. The enzyme can then be purified from the cells by various methods, and confirmed with sodium-dodecyl-sulfate polyacrylamide gel electrophoresis, activity assays, and optical density readings. The growth and purification of human adenovirus protease serotype 2 was conducted using *Escherichia coli* BL21 (DE3) cells transformed with a pET vector that was resistant to ampicillin and chloramphenicol, with the human adenovirus protease (AVP) gene ligated into it with restriction enzymes. Vectors were induced with Isopropyl b-D-Thiogalactopyranoside, lysed, centrifuged, and the supernatants were run through a Zinc column followed by an S-Sepharose column, purifying AVP. A considerable yield of 75% was obtained with very small amounts of DNA and other molecules in the background. This purification procedure can be applied repeatedly to use for future experiments utilizing pure AVP, or even for purifying other proteases similar in structure and amino acid sequence to AVP.

An Evaluation of Spill to Pass Juvenile Fall Chinook Salmon Through Columbia River Dams. ANN VEITZ (*Dakota State University, Madison, SD 57042*) DANIEL K. TANO (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Since dams have been built along the Columbia River, many different fish passage projects have been experimented with due to the decrease in chinook salmon populations due to migration route changes. One of these projects that have become a favorite in assisting juvenile fish passage was creating juvenile fish passage facilities and spilling water over the dams during fish migration season. Water flows are augmented at this time to both meet the need of the Power Administration and the Fish Passage Plan of 1977. There are seven facilities located at eight of the dams along the lower Columbia and Snake rivers where their fish guidance at the facilities have been found to be at 30%. Sampling efficiency studies have been performed at Ice Harbor Dam to determine how the juvenile fish respond to the facilities. Yet a difference comes about when there are high and low water years. The purpose of this study was to determine if the spill volume affects the passing of juvenile fall chinook salmon migrants at both John Day and McNary Dam using hatchery PIT tagged fish. Information about the detection dates/times were acquired along with the spill percents at each of the dams to help determine how many fish were actually using the juvenile facilities or the spill. Spills were found to be lower while detection rates were higher in 2001. Thus indicating that the fish were using the facilities. In contrast, the spills were higher while detection rates were lower in 2002. I conclude that the fish had a tendency of using the spill rather than the facilities during high flowing years.

Developing a PCR-Based Method to Genotype the Steel Panda (slp) Inversion. ROBERT WILLIAMSON (*The Colorado College, Colorado Springs, Co 80946*) YUN YOU (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Mouse chromosomal inversions are being used as balancer chromosomes in ENU (N-ethyl-N-nitrosourea)-induced mutagenesis projects at Oak Ridge National Laboratory. Recessive point mutations are generated in a regional-specific manner and they are maintained within a visibly marked inversion mutation. One of the inversion mutations used in the mutagenesis project is Steel-panda (slp), which carries a large chromosomal inversion spanning ~40 cM in mid-Chr10. A PCR-based method is needed to genotype the Slp inversion to facilitate the characterization of ENU-induced mutations. Toward this end, genomic clones overlapping the Slp inversion breakpoints were obtained. Based on the data from these clones, a PCR scanning strategy was employed to narrow the location of the distal Slp inversion breakpoint. This method defined the distal breakpoint within a 20 base pair region. After attaining this level of specificity with the distal breakpoint, Inverse Polymerase Chain Reaction (IPCR) was used in an attempt to clone a DNA fragment containing the distal slp breakpoint. The sequence of this DNA fragment can then be compared to wild type DNA to determine the location of the proximal breakpoint.

Purification Conditions and Crystallization Trials for Drosophila TATA Box-binding Protein Related Factor 2, dTRF2. TERESA WLASIUK (*University of California, Davis, Davis, CA 95616*) GERRY MCDERMOTT (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

TATA box-binding protein (TBP) is required for all three eukaryotic RNA polymerases to successfully recognize binding sites and initiate transcription. Tissue-specific versions of TBP have been identified. TBP-related factors (TRF1 and TRF2) bind to transcription factor IIA (TFIIA) and TFIIIB along with appearing as a subunit of a larger complex. TRF2 does not display TATA box-binding abilities that TBP and TRF1 show. We have overexpressed and purified a 227-residue construct that correlates to the core regions of TBP and TRF1. Crystallization trials for X-ray diffraction are in progress.

Habitat, Population Densities and Growth Metrics of the Asiatic Clam (*Corbicula fluminea*) Within Natural and Caged Environments in an Uncontaminated Stretch of the Hanford Reach, Columbia River. ANTHONY ZELINSKI (*Eastern Washington, Cheney, WA 99004*) BRETT TILLER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

At specific points in the Columbia River along the Hanford Nuclear Reservation (HNR) shoreline, contaminated ground water seeps into the river. This is a study of the natural demographics, such as population density and growth, of Asiatic Clams (*Corbicula fluminea*) at

an upstream (uncontaminated) location from the HNR. The objective of this study is to establish reference sites that will be useful for future researchers with similar studies at areas of concern on the HNR. The Asiatic Clam is a benthic, sessile organism that bioaccumulates Hanford derived contaminants. Those characteristics make this clam a good candidate for this study. Clam sampling was done via snorkeling and 0.1-m² submersible plot frames where densities, shell lengths and wet weights were recorded. Preliminary results show length frequencies of clams in the Hanford Reach of the Columbia River. Shell sizes ranged from 7-25 mm. Population mode was 14 mm. Population densities ranged from 460-1640 clams per 1-m² and had a mean of 792 with a standard error of 96 at the 90% exceedence level. These results are only from limited sampling but more sampling is currently being done. Future studies will be able to use this study as a reference or control to see if there is a difference, in the natural demographics of the Asiatic Clam, between areas of concern and reference sites.

CHEMISTRY

Solid State Cross Polarization, Magic Angle Spinning ¹³C Nuclear Magnetic Resonance Spectroscopy of Weakly-Coupled Organic Systems. COLE GOATER (*Coe College, Cedar Rapids, IA 52402*) E. W. HAGAMAN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Solid state Cross Polarization, Magic Angle Spinning ¹³C Nuclear Magnetic Resonance Spectroscopy (CP/MAS ¹³C NMR) has become a routine analysis tool among researchers in many fields. As use increases, especially for quantitative applications, the probability of insufficient attention to crucial parameters increases, particularly in analyses of proton-scarce compounds, in which many carbons have very weak 1H-¹³C dipolar interactions. The magnitude of the dipolar coupling determines the regulation error of experimental parameters required to prevent underestimation of carbon resonance intensities. The goal of this study was to measure the signal intensity responses of weakly coupled 1H-¹³C spin system containing organic substances as functions of MAS and ¹³C field amplitude. The effects of probe tuning under conditions different from those of the experimental acquisition were also assessed. Two systems were examined: Hexamethylbenzene (HMB) and Ill No.6 coal. HMB contains carbons with differing sensitivity in the CP/MAS experiment, making it a good model for evaluating parametric signal intensity dependence. Ill No.6 coal is a complex organic material, also containing a carbon fraction sensitive to the particulars of the CP/MAS ¹³C NMR experiment. Spectral response was assessed and expressed in terms of aromaticity (fa), the ratio of aromatic carbon intensity to total carbon intensity: $fa = Csp2/(Csp2+Csp3)$. A protocol has been developed, allowing optimum parameterization of the experiment. For these materials, the MAS speed and the 1H/¹³C field amplitudes need to be kept at 5000±125Hz and 85600±119Hz, respectively, to hold optimum performance.

A Study of Z-Scheme Photosynthesis. DANIEL HOLLAND (*Albion College, Albion, MI 49224*) JAMES LEE (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

A quantitative analysis of the Z-scheme theory of photosynthesis has been conducted in order to rigorously test the hypothesis. Studies were carried out on the algae strain *Chlamydomonas reinhardtii* 137c and various mutants of the strain: PS I-deficient mutants FUD26 and F8, and the PS I-deletion mutant B4-Psa A-D2. These studies included oxygen evolution measurements for photosynthetic rate determination, fluorescence-induction curves for relative quantum yields for the PS II reaction centers, and kinetic measurements of [P700] under weak actinic light for PS I antenna size calculations. In addition photospectroscopic measurements for PS I content, and pulsed-light H2 production yields (via the ferredoxin/hydrogenase pathway) were studied. Oxygen evolution at various light intensities was normalized to that of the wild-type algae and compared with the normalized product of relative antenna sizes and the amounts of PS I per chlorophyll. Relative O2 production rates of 0.56 (s = 28%) and 0.36 (s = 22%) for FUD 26 and F8, respectively, closely match H2 relative production of 0.55 (s = 24%) and 0.38 (s = 27%). Discrepancies exist between O2 and H2 production results and both the PS I content and antenna sizes, which are likely due to problems in the experimental design, as explained in the report. This work is fundamental research into the accepted model of photosynthesis. Although proposed long ago, a

thorough analysis with the many factors being simultaneously examined, and on the same samples at the same time, has not been pursued. Procedural and equipment modifications suggested by the authors should benefit future work.

Survey of New Calix[4]arene Aza-crown-6 Derivatives and Factors Affecting Cesium Extraction Performance. CARA JOHNSTON (*Colorado College, Colorado Springs, CO 80903*) LAETITIA H. DELMAU (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Four newly synthesized aza-analogs of the dioctyloxy-calix[4]arene oxo-crown-6 family were surveyed for their cesium, and more generally, alkali metal extraction performance. This study is part of an ongoing effort to clean up DOE tank-stored nuclear waste at sites such as Hanford and Savannah River. Selective removal of ¹³⁷Cs is of major importance as this radionuclide, along with ⁹⁰Sr, contributes 99% of the gamma radiation and heat generation of the waste. The new extractants contain two aza-substituents at the 3,4 or the 2,5 positions of the crown in either the free base form (NH) or the substituted form (NCH₂CH₂N₂Ts). The oxy analog of the compounds, dioctyloxy-calix[4]arene crown-6, was used for comparison. Alkali metal extraction performance was determined by either radiometric measurements or ICP analysis. Cesium extraction performance of each compound was measured as a function of pH, diluent, and anions present in the system. Results show an increase of the cesium extraction with pH. Diluent effects were consistent with the expected trends based on their properties. Cesium extraction from different sodium salt media followed the usual bias based on the anion free energies of partitioning. However, mixtures of dioctyloxy-calix[4]arene crown-6 with each substituted aza-compound showed a marked preference for hydroxide. Selectivity was on the order of 1000 for Cs over Na and on the order of 100 for Cs over K. The free base ligand behavior was analyzed by slope analysis to give the expected 1:1:1 cation:calix:anion stoichiometry. Overall, expected behavior was observed. Potential hydrogen bonding effects and interactive synergism need further investigation.

Protein Cross-Linking and Computational Techniques for the Identification of Protein Complexes. JANA LEWIS (*Lawrence University, Appleton, WI 54912*) GREGORY B. HURST AND JAMES L. STEPHENSON, JR. (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

By reacting with and connecting specific pairs of residues within a protein complex, chemical cross-linkers such as Bis(Sulfosuccinimidyl)suberate (BS3) can provide intermolecular and intramolecular distances in protein complexes. The goal is the identification of cross-linked fragments from a tryptic digestion of a protein complex and the assignment of distance constraints based on the length of the cross-linker spacer arm. The length of the cross-linker spacer arm is the maximum distance between cross-linked amino acid residues in the protein complex. A few cross-linked products per protein complex will provide enough low-resolution distance constraint information to eliminate inconsistent computational structure possibilities. Hemoglobin served as a model for developing a robust method of using cross-linking for high-throughput analysis of protein complexes. Lower protein and cross-linker concentrations were found to reduce the number of incorrect distance constraints. Fast Protein Liquid Chromatography improves the isolation of cross-linked products. Bovine hemoglobin lysine residues reacted with BS3 to form cross-linked products. The mixture of cross-linked and uncross-linked proteins was digested with trypsin and screened with matrix-assisted laser desorption/ionization mass spectrometry. Possible cross-linked products were further examined by electrospray ionization combined with Fourier transform ion cyclotron resonance (FTICR) mass spectrometry. Accurate masses supplied by FTICR mass spectrometry experiments provided a way to distinguish cross-linked fragments from hemoglobin tryptic peptides.

A Study of Z-Scheme Photosynthesis. CURTIS WEINRICH (*Northland College, Ashland, WI 54806*) JAMES W. LEE (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

A quantitative analysis of the Z-scheme theory of photosynthesis has been conducted in order to rigorously test the hypothesis. Studies were carried out on the algae strain *Chlamydomonas reinhardtii* 137c and various mutants of the strain: PS I-deficient mutants FUD26 and F8, and the PS I-deletion mutant B4-Psa A-D2. These studies included

oxygen evolution measurements for photosynthetic rate determination, fluorescence-induction curves for relative quantum yields for the PS II reaction centers, and kinetic measurements of [P700] under weak actinic light for PS I antenna size calculations. In addition photospectroscopic measurements for PS I content, and pulsed-light H₂ production yields (via the ferredoxin/hydrogenase pathway) were studied. Oxygen evolution at various light intensities was normalized to that of the wild-type algae and compared with the normalized product of relative antenna sizes and the amounts of PS I per chlorophyll. Relative O₂ production rates of 0.56 (s = 28%) and 0.36 (s = 22%) for FUD 26 and F8, respectively, closely match H₂ relative production of 0.55 (s = 24%) and 0.38 (s = 27%). Discrepancies exist between O₂ and H₂ production results and both the PS I content and antenna sizes, which are likely due to problems in the experimental design, as explained in the report. This work is fundamental research into the accepted model of photosynthesis. Although proposed long ago, a thorough analysis with the many factors being simultaneously examined, and on the same samples at the same time, has not been pursued. Procedural and equipment modifications suggested by the authors should benefit future work.

Synthesis of Novel Imaging Agents for Targeting EGF and ErbB-2 Receptors in Breast Cancer. LINDSY FARINA (*University of Alabama, Tuscaloosa, AL 35487*) HENRY VANBROCKLIN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*). Radio-tracer imaging agents for Positron Emission Tomography (PET) and Single Photon Emission Computed Tomography (SPECT) were synthesized in an effort to develop a non-invasive method for epidermal growth factor (EGF) and ErbB-2 receptor density determination in tumor cells. These receptors are overexpressed in many types of cancer, most notably, breast cancer. N-[m-Tri-(n-butyl)stannylphenyl] maleimide was synthesized and labeled with ¹²⁵I via iodo-destannylation. The resulting m-[¹²⁵I]IPM ((m-[¹²⁵I]-iodophenyl) maleimide) will then be conjugated to an ErbB-2 binding single chain antibody fragment via the highly reactive free sulfhydryl (thiol, -SH) group. The second branch of imaging agents explored was dialkoxyquinazoline analogs. These quinazolines were prepared by coupling dimethoxychloroquinazoline with 3 and 4-aminopyridines in DMF at reflux. Previous lead candidate quinazolines, labeled with either ¹⁸F (a positron emitter) or ¹²⁵I (a low energy gamma emitter), were used as radiotracers for the EGFR tyrosine kinase-binding assay. Development of these methodologies to produce new imaging agents may lead to more sensitive and more specific tracers for targeting tumor localization and monitoring treatment.

Relative Proton Affinities and Entropy of Protonation of Primary and Branched Alcohols Obtained From the Measurement of a Single Alcohol Pair. JOHN HACHE (*Creighton University, Omaha, NE 68178*) JULIA LASKIN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The kinetic method has proven useful for determining thermochemical properties of various compounds. In this study the usefulness of the kinetic method is investigated for branched alcohols, and the idea of the effective temperature is investigated. Where the traditional use of the kinetic method requires a series of bases to determine the thermodynamic properties of an unknown, this approach obtains such information from a single compatible pair of alcohols. Two transition state temperatures are determined for each alcohol pair and they are used to calculate the relative proton affinity and the change in entropy of protonation. Modification of the instrument was necessary to obtain accurate kinetic energy release distributions and the peaks obtained were smoothed and fit with a Gaussian curve. The presence of alternative reaction pathways was also investigated and is a suspected cause of the broadening of the peaks. The presence of these alternative pathways represents a limit of the kinetic method.

Determination of the Reducing Potential of Bacterial Cellulose and Sugar Incorporation During Growth. NATHAN WERNER (*Southern Utah University, Cedar City, UT 84720*) HUGH O'NEILL (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

It was discovered at ORNL that native purified bacterial cellulose produced by the bacterium *Gluconoacetobacter hansenii* catalyzed the precipitation of palladium from ammonium hexachloropalladate solutions. It was proposed that the aldehyde groups at the ends of the cellulose chains were responsible for this novel property of the material. The aim of this study was to determine the number of

reducing ends in a cellulose sample. An assay was developed to measure the number of reducing ends using the chromogen tetrazolium blue chloride that forms an insoluble blue diformazan when reduced. The data obtained indicated that at least one reducing end existed every 50 glucose residues. The incorporation of carbohydrates into bacterial cellulose was also investigated. Growth media that contained either glucose or fructose were inoculated with *G. hansenii*. Samples of media were taken directly after inoculation and after termination of culture growth. Cellulose produced by the cultures was cleaned and weighed. Each type of culture produced similar amounts of cellulose. It was calculated that on average 15.4% of fructose and 9.4% of glucose utilized by the bacteria, was incorporated into cellulose. Preliminary data indicated that the addition of ethanol or glycerol to fructose growth medium increased the proportion of sugar incorporated into cellulose with respect to that used in general cellular metabolism.

Application of Synchrotron Based XRF Microprobe to the Study of Ink and Paper. T.J. WILKINSON (San Francisco State University, San Francisco, CA 94000) DALE L. PERRY (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Analysis of paper and ink/paper combinations is essential to forensic science and law enforcement. Current analytical methods in use are destructive, and unable to provide result for small quantities of sample. In our work, synchrotron-based x-ray fluorescence microprobe has been used to analyze the low level metal ion components in commercial paper and commercial paper/ writing ink combined materials, and produce a 'metal fingerprint. Elemental maps for different metal ions are shown for blank paper and for ink that has been applied to and eluted on the same paper. Elemental analytical data for some of the common metal ions involved are presented, and the analyses for the metal ions in the ink/paper are discussed with respect to their origins and the processes and properties that are known for the paper.

Synthesis of Rotenone Derivatives: Mitochondrial Electron Transport Chain (ETC) Complex I Probes. LINDA XIONG (Fresno City College, Fresno, CA 93741) HENRY VANBROCKLIN (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The overall objective of the Department of Nuclear Medicine and Functional Imaging at LBNL is to develop efficient methods to help diagnose diseases and monitor treatment. The goal of this project was to produce new rotenone derivatives, compounds known to be potent inhibitors of the mitochondrial electron transport chain, which will be labeled with carbon-11 or fluorine-18 for PET (Positron Emission Tomography) imaging. These rotenone derivatives are potential imaging agents for cardiac diseases. Commercially available rotenone was converted into different analogs using various synthetic chemistry procedures. After each successful reaction step the product was purified and fully characterized. These compounds will be further converted to imaging agents in the radiochemistry laboratory or will be used to confirm the identity of the new radiolabeled compounds. Continuing the research towards finding new radiolabeled tracers will lead to better and more efficient means of identifying disease in the human body.

Determination of Gamma Radiation in Multiple Geometries. MICHAEL ALVAREZ (Harold Washington College, Chicago, IL 60605) ELANE STREETS AND VIVIAN SULLIVAN (Argonne National Laboratory, Argonne, IL 60439).

The different types of geometries and quantities of sample are a concern when being detected by an HPGe detector. Customers send samples that are in non-standard geometries, which causes somewhat of a problem when being analyzed by the HPGe detector. The detector is calibrated for full geometries and give results as if all geometries analyzed were full. Customers also send samples that do not have a sufficient amount of sample. A detector is calibrated for geometries that are full and correction factors are needed when a geometry is not full. Many different samples were analyzed at different heights and with different quantities so that correction factors could be calculated. The partially filled geometry and the samples at different distances away from the detector were analyzed and detected many different times to calculate the correction factors. The project concluded with a linear graph for the corrections factors to be used for non-standard geometries.

Mn Oxide Biogenesis and Metal Sequestration in the Presence of Co (II) and Cu (II) By *Bacillus* SG-1 Bacterial Spores. NADER BAYAT (University of California at Berkeley, Berkeley, CA 94720) JOHN BARGAR (Stanford Linear Accelerator Center, Stanford, CA 94025).

Mn oxides play an important role in degrading contaminants and cycling nutrients in soils and natural waters. The process in which Mn (II) oxidizes to form MnOx is slow; however, *Bacillus* SG-1 bacterial spores can catalyze the process and allow it to proceed up to five orders of magnitude faster. This experiment explored the affects of co-ion metal concentrations on Biogenic Mn oxide production and their ability to sequester metal cations. Spore solutions were prepared with different ratios of Metal (II): Mn (II) added over a four-week period; this was done separately for Co (II) and Cu (II). The copper solutions were analyzed by Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES) to check for the amount of copper and manganese left in solution after biogenic MnOx production. ICP-AES was used to analyze the ratio of Co: Mn in spores where Co was the co-ion metal. Observations showed that very little dissolved Cu and Mn existed in solutions with low copper concentrations, but large amounts of Cu and Mn were left in solutions in which higher Cu concentrations were used. This showed that high Cu concentration inhibited biogenic Mn oxide production and Cu sequestration. For the experiments with Co as the co-ion metal, it was observed that the ratio of Co: Mn in the spores was relatively similar to the ratios added; however, the exceptions to this rule were experiments in which high concentrations of Co were used. The inconsistency in Co: Mn ratios at high Co concentrations showed that high Co concentrations also inhibited biogenic Mn oxide production.

Nanoscale Photosynthesis and Artificial Vision: Generating Liposomes to Deliver Photosystem I to Inactive Retinal Cells. NOAH BELL (Williams College, Williamstown, MA 01267) ELIAS GREENBAUM (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Blindness due to the disease called macular degeneration is caused by the death of photoresponsive cells in the retina while the cells of the neural network that transmits the data from the eye remain intact. Photosystem I (PSI), a plant protein complex involved in photosynthesis, can generate voltages comparable to those needed for neural response. This creates the intriguing possibility of restoring vision in victims of macular degeneration by supplementing inactive retinal cells with PSI. One feasible method for delivering PSI centers to retinal cells is to deliver PSI by incorporating it into liposomes - enclosed bilayer lipid structures. However, predictably sized liposomes are needed in order to get PSI into the cells. A protocol was developed to produce such liposomes by extrusion, e.g., by forcing the lipid through 100nm pores under pressure. Both Atomic Force Microscopy and laser light scattering confirmed that the extruded liposomes had a narrow size distribution. Further characterization of the liposomes through the measurement of the phosphorous concentration in the lipid established that the developed protocol was both efficient and reproducible. Additionally, P700 bleaching tests confirmed that after their insertion into the extruded liposomes the PSI centers remained physiologically active. In comparison to previous methods of liposome production, the extrusion protocol was the most reliable method for the reproducible generation of liposomes of predictable sizes in a short time frame. Thus extrusion is recommended as the method for generating PSI-incorporated liposomes with predictable sizes and reproducible physiological characteristics.

Optimization of an Off-Line Chromatographic Fractionation Technique for Proteome Characterization by Mass Spectrometry. JOSHUA BLOSE (Allegheny College, Meadville, PA 16335) ROBERT L. HETTICH (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Proteomics is the study of the proteins expressed within an organism and includes the identification, characterization, and quantification of these proteins. Mass Spectrometry (MS) is a powerful technique for high-resolution characterization of biomolecules. However, to achieve optimum protein identifications, it is essential to fractionate this complex mixture prior to MS analysis. We propose a two-dimensional chromatographic approach to address this issue. The first dimension is an off-line anion exchange column fractionation of intact proteins using Fast Protein Liquid Chromatography (FPLC). The second separation

dimension is on-line with the mass spectrometer and utilizes reverse-phase liquid chromatography. The objective of this approach was to optimize conditions for the high-throughput fractionation of proteins with an anion exchange column, separating intact proteins based on their surface charge. We have optimized an FPLC fractionation method by loading 5-10 mg of soluble cell lysate on a 1 mL anion exchange column and collecting 28 1 mL fractions over 30 minutes against a linear 1M NaCl gradient. Each fraction contains approximately 100 proteins, an ideal condition for MS. Although fraction analysis by MS is unfinished, it appears that the objective of maximizing rapid protein fractionation with FPLC has been accomplished. For example, we have been able to measure more than 250 proteins at high resolution in two of the FPLC fractions from *E. coli*. Future work should include an evaluation of the efficacy of interfacing the FPLC on-line with the second dimension of reverse phase separation for higher throughput mass spectrometric detection.

Hydrogen Atom Abstraction Free Radical Kinetics from $\text{Fe}_2(\mu\text{-HS})_2(\text{CO})_6$ by Carbon Centered Radicals. THOMAS BÓWDEN (*University of St. Andrews, St. Andrews, SCOTLAND UK*) JAMES A. FRANZ (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The reactivity of the $\mu\text{-SH}$ bond, an important function in hydrodesulfurization and hydrogenase systems, was evaluated by studying the rate constant of hydrogen abstraction, k_{abs} from the organometallic iron compound $(\mu\text{-HS})_2\text{Fe}_2(\text{CO})_6$ and by comparing it with abstraction rates of 2-Mercaptonaphthalene, Octanethiol and other donors. Benzyl radical was formed by the photolysis of dibenzylketone in benzene. By observing the competition of hydrogen atom abstraction from $(\mu\text{-HS})_2\text{Fe}_2(\text{CO})_6$ by benzyl radical to form toluene versus benzyl radical self-termination to form bibenzyl, the rate constant for the hydrogen atom abstraction from the iron compound was calculated by using the expression: $k_{\text{abs}} = ([\text{To}]k_{\text{t}}/2)/([\text{BB}]1/2[\text{FeSH}]_{\text{av}} \text{deltat}^{1/2})$ giving $k_{\text{abs}} = 1.9 \times 10^7 \text{ M}^{-1}\text{s}^{-1}$. The Arrhenius expression for reaction of benzyl radical with $(\mu\text{-HS})_2\text{Fe}_2(\text{CO})_6$ is given by $\log(k_{\text{abs}}/\text{M}^{-1}\text{s}^{-1}) = 9.1 - 2.48/\theta$, $\theta = 2.3RT$ kcal/mol. These values are supported by B3LYP/LANL2DZ DFT electronic structure calculations for the isodesmic reaction, $(\mu\text{-HS})_2\text{Fe}_2(\text{CO})_6 + \text{HS} = (\mu\text{-HS})(\mu\text{-S}')\text{Fe}_2(\text{CO})_6$ predicting $\Delta H^\circ = -12 \text{ kcal/mol}$, leading to a bond dissociation strength of 78 kcal/mol, compared to a bond strength for the S-H bond of 88 kcal/mol. The activation of the hydrosulfido group by two Fe atoms is extraordinary, leading to a 100-fold enhancement in reactivity of the SH group in alkane thiols.

The Synthesis of Polycarbonates, Polyvinylferrocene, and Organometallic Complexes. HEATHER BROWN (*Columbia Basin College, Pasco, WA 99301*) TIM HUBLER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

This paper describes the synthesis of polycarbonates, polyvinylferrocene (PVF), and organometallic complexes. The work described herein relates to work accomplished during a ten week Community College Initiative fellowship at Pacific Northwest National Laboratory (PNNL). The three projects are: 1) synthesis of polycarbonates by direct insertion of CO_2 into oxetanes and epoxides followed by ring opening polymerization; 2) synthesis of PVF, an electroactive ion-exchange material, which is being developed for separation of pertechnetate ion (TcO_4^{1-}) from radioactive wastes and; 3) synthesis of organometallic complexes containing cobalt, which are remarkably efficient actinide extraction compounds. Project 1 offers background information for a possible alternative to current waste CO_2 disposal, while project 2 and 3 offer synthesis procedures specifically for the clean up of Hanford waste. The goals of this appointment were met as evident in new techniques learned from the above projects.

Nitroxy Catalyzed Oxidation of Carbohydrates. JOSEPH BULLOCK (*University of Kentucky, Lexington, KY 80503*) JOSEPH BOZELL (*National Renewable Energy Laboratory, Golden, CO 89401*).

The oxidation of several carbohydrates to the aldaric acid was carried out to explore the possibility of making industrial products from the dicarboxylic acid. The oxidations were carried out using the catalyst 4-acetamido-2,2,6,6-tetramethyl-1-piperdinyloxy (4-acetamido-TEMPO). The carbohydrates studied were d-glucose, d-galactose, d-mannose, d-xylose, and d-arabinose. The xylose derivative, 2,3,4-trimethoxy xylose was also oxidized to determine any change in the reactivity. What we observed was a much greater selectivity and yield in the six-

carbon sugars (i.e. glucose and galactose) than the five-carbon sugars (xylose and arabinose). Mannose is a six-carbon sugar that also gave poor yields. When applied to the trimethylated derivative, the oxidation gave a mixture of products in which there appeared to be no aldaric acid.

Analysis of Nitro-Aromatics and Nitro-Amines Via High Performance Liquid Chromatography (HPLC). DANIELLE COOK (*Sierra College, Rocklin, CA 95677*) AMRIT BOPARAI (*Argonne National Laboratory, Argonne, IL 60439*).

The Analytical Chemistry Laboratory (ACL) at Argonne National Laboratory is presently working on analysis of nitro-aromatics and nitro-amines in well water for an outside client. High-performance liquid chromatography (HPLC) coupled with a UV-Vis detector was used to separate, identify, and quantitate selected analytes in samples. All of the target analytes are used in either the production of explosives or degradation products of such processes. EPA method 8330 was used as a guide to set the parameters of the analysis. The detection limit for this method was approximately 1 ppb. Both low-level salting-out and solid-phase extraction (SPE) methods were used to prepare the samples for analysis. The HPLC had a 50:50 methanol water solution as the mobile phase and used a C-18 reverse phase column. Then a CN reverse-phase column was used to confirm results. The UV-Vis detector was set at 254 nm, a common setting for the absorption of both nitro-aromatics and nitro-amines. In this method, a calibration curve and the retention times of the target analytes were used to identify and quantitate the well water samples through statistical analysis. When choosing a method it is critical that investigators match the matrix of the sample to the matrix prescribed in the method, otherwise the results will not be as expected. The EPA methods can be tailored to fit different needs; however, the results will be different and will not meet EPA standards. HPLC is a good analytical tool for analysis of nitro-aromatics and nitro-amines in water.

Refining Refinement: Benefiting from Awareness of the Incomplete Model in Computational Crystallography. AREL L. CORDERO (*University of Oregon, Eugene, OR 97403*), PAUL D. ADAMS (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Determining the three dimensional structure (tertiary structure) of protein molecules is the primary goal of protein X-ray crystallography. Computational techniques are critical to the construction and refinement of a model that best fits the experimental data. An important component of the model is the disordered solvent region of the crystal, or bulk solvent, which is accounted for by a constant electron density level outside the protein. Unfortunately, current methods also treat residual electron density from an incomplete protein model as part of the bulk solvent. In this research, methods were tested in which these two components were treated independently in both refinement and the creation of electron density maps. Forty-three solved protein structures, with diffraction resolution ranging from 3.5 to 1.1 Å ($1 \text{ Å} = 10^{-10} \text{ m}$), were used for testing and comparing the methods. Randomly selected regions of 2.5, 5.0, 7.5, and 10% of the models were removed from each protein and the models were refined using the new and current methods. Electron density maps were calculated from the models and observed data. Correlation coefficients between the electron density maps calculated from the incomplete models and the final structure were calculated and compared. The best of the new methods for treating an incomplete model demonstrated a measurable improvement over the current method and the improvement increased as the percentage of the model missing increased. This new method will be particularly important in the early stages of iterative automated model building where very incomplete models must be refined and electron density maps calculated for the next cycle of building.

Characterization of Functionalized Carbon Nanoloop-Antibody Structures as Membrane Probes. CORY DAIGNAULT (*Florida State University, Tallahassee, FL 32306*) JOHN WARREN (*Brookhaven National Laboratory, Upton, NY 11973*).

Carbon nanotubes have recently attracted considerable study in the scientific community due to their unique structure dependent, mechanical and electrical properties. Thus far their applications to biology have been limited, though their robust nature has many potential applications. This investigation focuses on the functionalized nanoloops by attaching monoclonal antibodies for the gC1q-R receptor protein (74.5.2 and 60.11) to the surface of nanoloops, ring-shaped single-

walled carbon nanotubes. Atomic force microscopy (AFM) and transmission electron (TEM) microscopy were used to characterize the protein functionalized carbon nanotubes loops. The loops were made by treating single walled nanotubes (SWNT) with acid, heat, and sonication in the presence of H₂O₂. These chemically cut tubes were treated with carbodiimide to form loops and attach the biological proteins. The average widths of the functionalized loops ranged from 25-36 nm and the heights ranged from 1.6-3.0 nm. The height value reported refers to the material trapped and apparently bound in the central cavity, for the loops with protein treatment. These nanoscale complexes have a size that can be seen using AFM and TEM. Due to these properties, the antibody-nanoloop complexes may provide for delivery systems for doing dynamic living cellular experiments.

Initial Studies Concerning Minute Deflections of Nuclear Isomers in an Inhomogeneous Magnetic Field. ANTHONY FITCH (*University of Nebraska Kearney, Kearney, NE 68849*) BOB W. SHAW (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*). Nuclear isomers are an area of high interest due to the fact that certain isomers have a high energy density that could be used to produce energy on a large scale. Investigations are underway about how to release the energy, but due to the fact that the isomers are only produced on the scale of parts per million, a method of enrichment is needed. The method proposed by R.W. Shaw, is to pass a beam of atoms through an inhomogeneous magnetic field and separate the isomers from the ground state nuclides based on their magnetic moment. A summary will be presented of the preliminary studies for a continuous beam process in which an ion beam is first passed through a mass selector, decelerated, neutralized in a cesium cell, and then passed through the inhomogeneous magnetic field. These preliminary studies tend to show that there is too much divergence in the beam and most of the atoms would not make it through the magnet. There would be better throughput if the ions were collected and neutralized after the mass selector and then evaporated in an oven and passed through the magnet.

D-threo-methylphenidate Induced Increase in Striatal Dopamine Unaffected by l-threo-methylphenidate Pretreatment. SARA GONZALEZ (*University of Scranton, Scranton, PA 18510*) and SUZANNE HULME (*McGill University, Montreal, QC H3A2T5*) MADINA GERASIMOV (*Brookhaven National Laboratory, Upton, NY 11973*). Each year, millions of patients diagnosed with attention-deficit hyperactivity disorder (ADHD) are treated with methylphenidate (MP, Ritalin®). Methylphenidate is marketed as a racemic mixture of l-threo-methylphenidate (l-threo-MP) and d-threo-methylphenidate (d-threo-MP). The d-threo form works by selectively blocking dopamine (DA) transporters and increasing synaptic DA concentrations. The l-threo form has been thought to have no significant effect on DA. In this study, microdialysis and high-pressure liquid chromatography (HPLC) were used to investigate whether l-threo-MP attenuates the dopaminergic effects of d-threo-MP when administered 15 minutes prior to the pharmacologically active enantiomer. Effects of MP were evaluated as a function of the change from the basal levels of extracellular DA in the corpus striatum of the rat brain. Three groups of 250-300g rats were treated with 5.0 mg/kg of d-threo-MP administered intraperitoneally. One group of animals received no other treatment, another group received a saline injection 15 minutes prior to injection with d-threo-MP, and a third group was injected with 5.0 mg/kg l-threo-MP 15 minutes prior to injection with d-threo-MP. Pretreatment with l-threo-MP resulted in a mean initial DA increase of 362% 15 minutes following the administration, which was not significantly different from the mean initial increase demonstrated in the group with no pretreatment (471%, $p=0.196$, two tailed t-test) or in the group pretreated with saline (431%, $p=0.489$). This evidence suggests that the l-threo enantiomer does not reduce the efficacy of the active d-threo form.

Scientific Software Development in the 21st century: Tools for Solving the Scientific Challenges of Tomorrow, Today. MARY GRIFFIN (*Vassar College, Poughkeepsie, NY 12604*) WILLIAM A. LESTER, JR. (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

This project involved the creation of a complex ab initio quantum mechanics package for performing quantum Monte Carlo calculations of the electronic structure of atoms and molecules. Specifically, a variety of electron-electron and electron-nuclear correlation functions for electronic wave functions was added to the package. Several of

the important tools of the computational chemistry and physics community are used. This paper will review some of the freely or widely available software tools for computational chemistry and how they are the loom in which the new generation of scientists weaves the tapestry that is the software of tomorrow. In addition, the use of electronic correlation functions within a developing software package is explored. The purpose of implementing this part of the program is to evaluate the utility of various proposed correlation functions for use in quantum Monte Carlo simulations of large molecules. Once this is successfully completed, the correlation function parameters will be optimized and the variance of the local energy will be calculated for systems of various sizes. Since the smallest variance of the local energy indicates the most accurate trial wave function, this work will provide a benchmark against which one may determine the type of correlation function within the trial wave function that is best suited for larger systems than those treated to date with the method.

Homogeneous Photocatalysis: Splitting Water into Hydrogen and Oxygen Using Visible Light in the Presence of the Photocatalyst-catalyst, Tris(dithiolene) Tungsten. KAYLI HALL (*Creighton University, Omaha, NE 68178*) S. THOMAS AUTREY (*Pacific Northwest National Laboratory, Richland, WA 99352*).

In this technological age, energy, necessary for fueling a majority of daily activities, is often taken for granted. As nonrenewable sources of energy such as petroleum and coal become depleted, the search for a clean, renewable energy source becomes imperative. Scientists have turned to molecular hydrogen as the next great energy provider, especially in the realm of fuel cell technology. If hydrogen can be isolated from renewable resources such as water and sunlight, a major step toward solving the energy crisis could be realized. In an in-situ attempt to quantify and reproduce results that demonstrate the isolation of molecular hydrogen by exposing water to visible light from studies conducted at the University of Athens, Greece, pre-purified water was exposed to a 1000W Xenon-Mercury lamp in the presence of an isolated isomer of the photocatalyst-catalyst (PCC) Tris(dithiolene) tungsten compound and methyl viologen. No sacrificial donor was needed for this process, and hydrogen production was measured using mass spectroscopy and gas chromatography. Experiments were also conducted using deuterium oxide to show the exact source of the hydrogen. In both cases, neither hydrogen nor deuterium was produced. Current studies show that this may be the result of trace impurities from the glassware. Steps, therefore, are being taken to institute a rigorous cleaning procedure for the photochemical reactor used to isolate hydrogen. In the future, steps may be taken to analyze the mechanism by which water is split into hydrogen and oxygen in the presence of visible light and ultimately, optimize this process.

Experiments in Growing Patterned Nanophase Diamond Thin Films. ANDREW HERR (*Rensselaer Polytechnic Institute, Troy, NY 12180*) ROBERT W. SHAW (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Steps were taken toward the creation of corrugated nanophase polycrystalline diamond thin films. These films have potential as stripper foils for the H- beam in the front end of the Spallation Neutron Source (SNS). Preliminary tests have shown that diamond films have a much longer lifetime in this application than conventional carbon stripper foils. Some flat films were prepared for a simulated beam test at Brookhaven National Laboratory by etching the silicon substrates away from the films to create diamond windows. Geometric limitations mandate that the films in the SNS can only be supported on two adjacent sides of a square window. Because residual stresses cause flat films to curl when unsupported, attempts were made to grow corrugated films for more mechanical structural integrity. Hot filament chemical vapor deposition (HFCVD) was used to grow one-micrometer thick films on patterned silicon substrates. The substrates were patterned using photolithography to produce roughly 20-micrometer tall ridges running diagonally toward the freestanding corner of the film. The substrates were characterized using a surface profiler as well as a scanning electron microscope. Limited success has been achieved at getting conformal films to grow in the troughs between the ridges in a one-micrometer film. Experiments on how to increase growth in the troughs were performed including etching patterned substrates further and varying scratching techniques. Also, a microwave plasma CVD system was installed and configured for use and a few films were grown in it. In theory this new system will create larger, more uniform films.

Semi-Volatile Organic Compounds in Seattle Air, Part II: Improving Productivity and Accuracy in Data Analysis for High Performance Liquid Chromatography. CLINT HOBERG (*Pima Community College, Tucson, AZ 85709*) LARA GUNDEL (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Understanding human exposure to airborne polycyclic aromatic hydrocarbons (PAH) requires accurate measurements of their partitioning between the gas and particulate phases. The difficulty of measuring this partitioning efficiently and accurately has been an area of major concern. Prior methods involving GC/MS had left out many PAH due to poor sensitivity. Fluorescence detection with high performance liquid chromatography (HPLC) has greater sensitivity but the HPLC manufacturer's software produces data that can be so noisy that limits of detection suffer unless the analyst inspects and analyzes each chromatogram manually. This is a very time consuming process that limits sample throughput. The objective of this project was to adapt a commercially available software product, PeakFit, for the analysis of PAH fluorescence data for automatic rather than manual processing of each chromatogram. The software used a Fourier deconvolution method as well as a Loess smoothing routine to prepare the data for further analysis. Fourier deconvolution was used because the fluorescence detectors have a zero order (true linear) response factor. We found that analysis time decreased five-fold, for a productivity increase of 5. Accuracy also improved because the software could be adapted to locate and quantify peaks that were poorly resolved. In comparison to the manual reference method PeakFit had a relative r2 value of around 0.99 for the compounds of interest, compared to r2 of about 0.5 for the same group of PAH as quantified by the HPLC software package. With these improvements LBL will be able to report Seattle PAH concentration and gas/particle partitioning data by the end of 2002.

Analyzing Xanthine Dehydrogenase Iron-Sulfur Clusters Using Electron Paramagnetic Resonance Spectroscopy. RACHAEL HODSON (*Oklahoma State University, Stillwater, OK 74078-1012*) GRAHAM N. GEORGE (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

Xanthine dehydrogenase is a metalloenzyme that is present in a variety of eukaryotic and prokaryotic organisms. The oxidation of the xanthine occurs at the molybdenum site, and the catalytic cycle is completed by electron transfer to the iron-sulfur (Fe/S) clusters and finally the flavin, where they are accepted by nicotinamide adenine dinucleotide (NAD). Since the site giving rise to the Fe/S I electron paramagnetic resonance (EPR) signal is thought to be the initial recipient of the electrons from the Mo, we wish to understand which EPR signal is associated with which Fe/S cluster in the structure in order to develop an understanding of the electron flow within the molecule. Samples of xanthine dehydrogenase wild-type and mutant forms were analyzed with EPR spectroscopy techniques at low and high temperatures. The results showed an altered Fe/S I signal along with an unaltered Fe/S II signal. The converted Cysteine, in the mutant, did affect the Fe/S cluster immediately adjacent to it. Therefore, the Fe/S I signal arises from the Fe/S cluster closest to the Mo and immediately adjacent to the mutated amino acid, and the Fe/S II signal must arise from the more distant Fe/S cluster.

Optimization of Solvent Extraction of bis-(2-ethylhexyl) Phosphoric Acid (D2EHP) from Aqueous Environments. MARY HULTGRENN (*Whitworth College, Spokane, WA 99301*) JAMES A. CAMPBELL (*Pacific Northwest National Laboratory, Richland, WA 99352*).

During the processing of nuclear materials by solvent extraction with tributyl phosphate and ion exchange with both anion and cation exchange resins resulted in high-level waste. The radioactivity present in the tank wastes has contributed to degradation of a variety of organics. These include dibutyl phosphoric acid, trimethylamine, and other organics. D2EHP is an organic that is present in tank waste because it was used as an extractant in Sr recovery. The need to identify and analyze all of these organics is necessary. Extracting waste materials with ethyl acetate separates organic compounds. After extraction, derivatization with diazomethane is performed. The analysis of the extracted solvents from other tank waste materials is done by gas chromatography/mass spectrometry (GC/MS) and gas chromatography/ flame ionization detection (GC/FID). The results proved that extraction with ethyl acetate and derivatization with diazomethane is most effective in separating phosphates.

Studies of the Surface Charge Properties of Titanium, Aluminum, and Uranium Oxides by Potentiometric Titration. CHRISTINA LEGGETT (*Florida State University, Tallahassee, FL 32313*) HEINO NITSCHKE (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The reprocessing and separations of radioactive wastes in soils is a major concern in nuclear industry. An understanding of the surface properties of these actinide components, in the form of oxides, can facilitate removal of these actinides from soils and prevent their migration through the geosphere. Potentiometric titrations of titanium and aluminum oxide in aqueous media of different ionic strengths were conducted to determine the point of zero charge. Experiments conducted with titanium and aluminum oxide were for method development. The point of zero charge (PZC) of TiO₂ in 0.001 M, 0.05M, 0.01M and 0.1M NaClO₄ systems was calculated as 6.05 ± 0.147. Aluminum oxide titrations in 0.001 M and 0.01 M NaClO₄ solutions yielded a PZC value of 9.27 ± 0.0353. The point of zero charge for U₃O₈ is 8.61. The uranium oxide data will prove to be an invaluable annex to the literature data as no data is available on this oxide.

Sample Preparation Methods for Analysis of Airborne PAH. RACHELLE MAJESKE (*Crafton Hills College, Yucaipa, CA 92374*) LARA GUNDEL (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The objective of this project was to devise sample preparation methods for analysis of airborne PAH in samples of particulate matter collected in Seattle in 2001. Existing methods for hexane extracts were improved to isolate non-polar PAH from extracts in a mixture of hexane, dichloromethane and methanol. These contained both non-polar and polar organic compounds. The new method also had to increase productivity in the lab while minimizing analytical errors. Sample extract cleanup (removal of interferences) and solvent change steps were accomplished using a single silica solid phase extraction column instead of two. Changing solvent from hexane to acetonitrile for compatibility with reversed phase HPLC was carried out during evaporation, by taking advantage of the different boiling points of these two solvents. By eliminating certain steps and shortening others, the processing time was reduced by a factor of three. The new procedure was validated in quadruplicate by processing a mixture of standard PAH as a surrogate for extracts of PM. Recoveries averaged 91.6 ± 2.6%, confirming the efficacy of this new method.

Synthetic Methods and Administration of [11C]Acetone For Positron Emission Tomography. RYAN MULLER (*College of William and Mary, Williamsburg, VA 23186*) STEPHEN L. DEWEY (*Brookhaven National Laboratory, Upton, NY 11973*).

As acetone has become an increasingly abused inhalant worldwide, researchers have developed a radiotracer form of the compound, [11C]acetone, for positron emission tomography (PET) studies. Since the synthetic scheme for [11C]acetone calls for the rapid delivery of ¹¹C to an isolated reaction vial, a system was designed to trap and release ¹¹C from cyclotron target gas without the moisture condensation difficulties of cryogenic trapping. Beyond the target gas trap, a valve-operated reaction panel was constructed and has successfully generated radiochemically pure [11C]acetone for PET imaging. This radiotracer has since been administered to an anesthetized rat and imaging results demonstrate high uptake in the brain. Pharmacokinetic analysis indicated an 8-minute washout half-time in the striatum and cerebellum. Encouraging results from these initial imaging studies indicate the potential for [11C]acetone to be imaged further in primate and human protocols.

Synthesis of a Novel Boron-Containing Porphyrin. JARED NIED (*Long Island University, Southampton College, Hampton Bays, NY 11946*) MICHI MIURA (*Brookhaven National Laboratory, Upton, NY 11973*).

Glioblastoma multiforme is a virulent, aggressive type of brain cancer that arises from the astrocytes that for the blood-brain barrier and protect the brain's neurons. GBM is so malignant and lethal that the median survival time after diagnosis is a mere 8.6 months, with a totally negligible percent of patients surviving to 5 years. Conventional treatments, consisting of surgery to remove most of the tumor mass and radiation therapy to attempt to kill any remaining cells, shows little if any promise of extending survival times. A promising possible therapy for these types of cancer is boron-neutron capture therapy, which is a bimodal therapy consisting of a boron-10 containing

compound and a beam of thermal neutrons. When the neutrons encounter the boron-10, the boron splits into a lithium-7 nucleus, an alpha particle, and gamma radiation. The damage that these particles cause is entirely confined to the cell containing the boron. If boron compounds are selected that will preferentially accumulate in tumor cells, the therapy will prove extremely lethal to those cells, while leaving healthy tissue unscathed. Since it does not contain boron, the neutrons pass through it uneventfully. Porphyrins are one class of chemical that has been found to selectively uptake into tumor cells. This project focuses on the total synthesis of a novel boron-containing porphyrin for BNCT.

Synchrotron Structural Approaches to the Chemistry of Metal Ion-Imidazoles. MARIO ORTEGA (University of California at Davis, Davis, CA 95616) DALE L. PERRY (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

In the chemical world there are thousands upon thousands of bioinorganic compounds which have been identified, but have not been significantly analyzed for their important relevant properties and possible uses. The process of creating new drugs, materials, and semiconductors relies on the reactions of two or more substances to create a more complex one. Understanding the importance of this concept and utilizing are what enable breakthroughs to be made in many of these fields. During my time at LBNL I synthesized several imidazole compounds and the structural data was analyzed through the X-ray Crystallography beam line 11.3.1 of the Advanced Light Source. With the aid of this instrument I was able to see the atomic structure of my crystals and adjust my synthesis accordingly to attempt to eliminate impurities and attain the imidazole structure. The imidazole structure would not crystallize, leaving me with crystal structure data of imidazole compounds. Imidazole and related compounds constitute the backbone of histidine and many peptides involved in human biological processes. With the data of these types accumulated here, some previously unexplained biological chemistry and related phenomena may one day be known.

Modification of FORTRAN Code to Analyze Data of Pulse Radiolysis Method. BHAIK PATEL (Rutgers University, Jersey City, NJ 07307) JOHN MILLER (Brookhaven National Laboratory, Upton, NY 11973).

Long-distance electron transfer has been studied in several systems in which D and A have been kept apart by a rigid spacer group or by incorporating them in rigid glass or polymers. Recent crystallographic work and kinetic measurements on photosynthesis reaction centers have shown that nature makes use of LDET in one of the most important processes known, photosynthesis. Our research involves the synthesis of suitable molecules, tailor-design to measure intermolecular electron-transfer rates of the type $A1 \text{ } ^{-} \text{ Sp } ^{-} A2 \text{ } ^{-} A1 \text{ } ^{-} \text{ Sp } ^{-} A2$ where A1 and A2 are group with finite electron and Sp is a rigid spacer with no electron affinity of its own. The experiment involves the generation of negative radical ions from the molecules by pulse radiolysis and the kinetic measurement of the intermolecular electron-transfer rates establishing equilibrium by optical absorption. This chemical reaction is measured by passing radiation beam light through mixture. In this experiment, chemical reaction happens within nanoseconds or Picoseconds over the time period, and this data are collected in VAX machine to observe the result by using FORTRAN code. This code execute on legacy Vax system. Plotting and graphing data hauling of data require detail instructions (calls). This problem resolved by using IGOR software, which especially made for research purpose and has constructive options like graphics, procedure window, built in functions.

5-Volt Cathode Materials for Lithium Batteries. XIAOQING QIAN (Washington University, St. Louis, MO 63105) CHRISTOPHER JOHNSON (Argonne National Laboratory, Argonne, IL 60439).

A modified sol-gel method was used to prepare a series of X metal substituted 5-V spinel oxides. The standard, undoped spinel oxide $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and its doped derivatives, $\text{LiNi}_{0.4}\text{X}_{0.1}\text{Mn}_{1.5}\text{O}_4$ (X=Cr, Zn, Fe, Al, Mg, Ga, V, Cu), were successfully synthesized and their structures verified with X-ray diffraction (XRD) measurements. Electrochemical performance was evaluated with Li coin cells in the configuration: Li/electrolyte/ $\text{LiNi}_{0.4}\text{X}_{0.1}\text{Mn}_{1.5}\text{O}_4$ between the voltage limits 3.5 to 5.0 V. Specific discharge capacities of about 130 mAh/g were obtained with good reversibility. The voltage profiles indicate a two-electron redox process at the Ni metal center occurs over two

plateaus at about 4.7 - 4.6 V, while a small shoulder related to either the Mn or the X metal redox process is observed at about 4 V. Results suggest that these types of materials will be very useful in new batteries engineered to operate at 5 V in a Li battery.

Investigation of Electromagnetic Spectrum of HCB[•] Radical. PINTO ROSANGELY (University of Puerto Rico, Cayey Campus, Cayey, P.R. 00736) SEARS TREVOR (Brookhaven National Laboratory, Upton, NY 11973).

Bromomethylene (HCB[•]) is a reactive species belonging to the carbene (divalent carbon containing compounds) family. It is formed as a short-lived intermediate in the burning of bromine-containing fuels and in the chemistry of the polluted atmosphere. Spectroscopic methods may be used to monitor the presence and concentration of this species in chemical reaction systems, and we reported the observation and rotational analysis of part of the visible spectrum of the radical for the first time. HCB[•] was made by photolysis of bromoform (CHBr₃), in an excess of Helium in a slow-flow gas mixture, at 193 nm using a pulsed excimer laser. The HCB[•] radical was detected by the absorption of single frequency continuous-wave dye laser pumped by an Argon ion laser. The weak absorption lines were measured using frequency modulation of a dye laser beam followed by demodulation of the signal from a fast photodiode detector monitoring the transmitted laser beam. The spectrum was measured relative to the well-known spectrum of iodine and the line positions were estimated to be accurate to within 0.02 cm⁻¹. Approximately 100 rotational lines in the 060 '000 band (here the numbers correspond to the three vibrational quantum numbers in each electronic state) were assigned. Their positions were used to determine the upper state rotational energy levels and thereby estimate the structure of the radical in this state. These results will be useful for future studies of chemical reactivity of this species and for monitoring the radical in chemical reaction systems.

Electronic Properties of Carbon Nanotubes. MONICA SAMEC (University of Toronto, Toronto, ON M5S 3G3) RANDY ELLINGSON (National Renewable Energy Laboratory, Golden, CO 89401).

Single-walled carbon nanotubes (SWNTs) have unique properties that lend themselves to many potential applications. In order for nanotubes to reach their full potential, it is necessary to have comprehensive understanding of their electronic properties. However, acquiring this knowledge presents major challenges. A nanotube's thermal, electrical, and physical properties vary significantly with its diameter and chirality. Since it is not yet possible to synthesize a specific type of nanotubes, scientists must work with samples of many nanotubes with different properties. In this experiment, laser deposition was used to synthesize SWNTs at different pulsewidths. The material was then purified and cast into a 0.1% m.w. film using a Nafion polymer. The UV-Vis-NIR spectra of the samples were analyzed, and no significant differences in absorbance regions were found. Long- and short-range dynamical spectra of the 2 is pulsewidth sample were analyzed. A double exponential curve was fit to the initial ultrafast decay and a single exponential was fit to the slower decay. Based on the dynamics observed in other nanomaterial systems, the faster decays may be attributed to charge carrier cooling and delocalization of charge along the nanotube, and the slower decay may be due to electron-hole recombination. In these measurements, the decay attributed to charge carrier cooling becomes slightly more influential at a higher energy probe pulse.

Coupling Thin Layer Chromatography and Electrospray Mass Spectrometry via a Surface Sampling Probe Interface. AMAURY SANCHEZ (Florida International University, Miami, FL 33199) GARY VAN BERKEL (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Coupling thin layer chromatography (TLC) and electrospray mass spectrometry (ESMS) provides a method of separation, detection and structure determination. A complex problem in combining TLC and MS is lack of a suitable interface to directly sample material from the plate surface without the requirement of a lengthy preparative process. Using a surface probe interface provides a reasonable and efficient solution. Matrix assisted laser desorption ionization (MALDI) directly analyzes TLC plates, but stringent conditions (e.g. vacuum and non-standard TLC plates), matrix requirements, limited detection of low mass analytes due to extensive matrix background ions, and pre-MALDI plate preparation limits this method. A dye mixture (made up of three components) dissolved in methanol was developed in 60:40

Methanol/Tetrahydrofuran with ~ 0.100 g of ammonium acetate on a reverse phase TLC plate. After a period of drying (air or oven), the MS directly analyzed the plates. Three main areas studied were: 1) Detection levels. 2) Stepwise sampling of surface at regular intervals. 3) Scanning using a liquid junction between plate and probe. An X,Y,Z manipulator was used to automate scanning and stepwise surface sampling. Picomol detection and a high degree of spatial resolution were obtained from this technique. Through implementation of a surface probe interface and using the electrospray ionization method, the plate surface can be directly analyzed with greater speed and ease.

Urea Reactions With Rare-Earth Metal Ions. JACK SARKANY (*Las Positas College, Livermore, CA 94577*) DALE L. PERRY (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Urea is a basic important biological organic compound. Urea is essential in all of the ecosystems in the world. Detection of this compound is essential in the way we analyze samples. Instead of separating the sample, a simple detection of urea can be made possible with relative ease, and in a safe manner. Metal oxides help in making complexes with urea and other metal ions. With a metal base, the sample can be mixed with a rare-earth metal ion and then splashed onto a sample; being able to be seen with IR analysis. This simpler IR spectrum can be compared to the original rare-earth metal ion, and prove or disprove the appearance of urea or not.

Synthesis of N-Alkylaza-21-Crown-7 Ethers For Purposes of Cesium Extraction from High-Level Waste. STEPHEN SCHAYER (*La Salle University, Philadelphia, PA 19141*) LAETITIA DELMAU (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Studies toward the synthesis of new azacrown-ether molecules were carried out by utilizing and modifying a suggested reaction scheme. Recent studies have suggested that Cs⁺ may bind strongly to a 21-crown-7-ether containing a nitrogen-donor atom in place of an oxygen-donor atom because of an improved dipole orientation. The crystal structure of the free ligand, N-ethylazatribenzo-21-crown-7, seemed promising for binding cesium; however, the ligand was only synthesized in minute quantities. A larger-scale, multi-step synthesis involving the making of a tribenzodiphenol with two protecting tosyl groups, followed by a deprotection to obtain the phenol groups, and then ring-closure using dichloroethamine was attempted. The first step quantitatively yielded the desired compound. The deprotection was found to be a fairly non-reproducible reaction. Multiple attempts consistently yielded a mixture of products not easily separated by regular separation methods, such that a new reaction had to be introduced: the mixture of products was reacted with magnesium in dry methanol to exclusively yield the deprotected diol. With this necessary modification, the synthetic scheme is expected to proceed and yield N-alkylazatribenzo-21-crown-7 ether. While this tribenzo crown ether was the target compound because of its rigid structure preorganized for cesium extraction, more flexible dibenzoazacrown ethers derived from diols already available were also under synthetic investigation.

Studies of the Thermal Stability of Metal Fuels Containing Plutonium, Zirconium, Americium, and Neptunium Using DSC-TG. JENNIFER SLOPPY (*Indiana University of Pennsylvania, Indiana, PA 15701*) J. RORY KENNEDY (*Argonne National Laboratory, Argonne, IL 60439*).

The Accelerator Transmutation of Waste (ATW) project aims to recycle spent fuel from light water reactors into usable blanket fuel. These recycled blankets would contain higher actinides such as Pu, Am, and Np which would be transmuted to short-lived or stable isotopes when used as blanket fuel. Unfortunately the properties of such fuels are unknown. Using differential scanning calorimetry-thermogravimetric analysis (DSC-TG), experiments conducted on transmuted alloy fuels showed that no measurable volatilization or melting of the fuel occurred. Phase transitions were observed for Pu and Zr. The transitions observed at approximately 515°C and 700°C may be due to changes in the Np-Zr phase.

Experimental Design, Synthesis and Characterization of Cyclobutene for Photofragment Translational Spectroscopy Studies at 193 nm. ABRAHAM SPENCE (*University of Rochester, Rochester, NY 14627*) DANIEL M. NEUMARK (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Over several decades, research has brought much attention to the photochemistry of unsaturated hydrocarbons, which has led to many astounding advancements in our understanding of these processes. Such developments include the elucidation of the photodissociation dynamics of a given molecule, more specifically, hydrocarbons existing with at least one degree of unsaturation. Photofragment Translational Spectroscopy (PTS) has previously been used to investigate the dissociation dynamics of such molecules as 1,2-butadiene and 1,3-butadiene with great success. Among such a vast amount of information, further studies have developed concerning molecules, which behave similarly to those previously investigated. Cyclobutene, a high energy unsaturated hydrocarbon, has become a valid candidate due to its potential similarities in transition states and intermediates formed during its dissociation when compared to many of those previously investigated. In order to be utilized in PTS studies, a high purity synthesis was developed to successfully yield the gas phase product. Furthermore, a single synthesis must yield a sufficient amount of product to complete the entire study due to the large hindrance that impurity exhibits. Due to this fact, the reaction between bromocyclobutane and potassium hydroxide in ethanol must be carried out in high yield utilizing a custom designed vacuum apparatus. Characterization must then be performed to ensure cyclobutene, the desired product, was synthesized in high purity. Subsequently, PTS studies will then be used to investigate the dissociation dynamics of cyclobutene leading to a thorough comparison of the results to that of previous studies.

13C Spin-Lattice Relaxation Time Measurements of Benzene in Small Pores. KARL STUPIC (*Juniata College, Huntingdon, PA 15745*) EDWARD W. HAGAMAN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

This project is part of a study of the motion of molecules, in confined spaces. Benzene was placed in Vycor (porous glass) to create this environment. Motion was monitored by measuring C13 spin-lattice relaxation time. There are three major areas of data collection: (1) T1 (Spin-Lattice) Relaxation of bulk benzene (proton and deuteron, both in air and degassed), (2) T1 of benzene in Vycor glass cylinders, (3) T1 of a monolayer benzene adsorbed onto the surface of the Vycor glass. Cross-polarization was attempted to detect a single monolayer out of the bulk solution and measured its T1. Cross-polarization loses its strength as a function of the distance between the two atoms. The cross-polarization rate falls off as the negative sixth power of that distance, and limits detection to about 5 D from the cross-polarization source (silanol protons).

Synthesis of [11-C]Nisoxetine for PET Study of Norepinephrine Transporters. DAVA SZALDA (*Syracuse University, Syracuse, NY 13210*) YU-SHIN DING (*Brookhaven National Laboratory, Upton, NY 11973*).

Positron Emission Tomography (PET) is a valuable medical imaging tool in studying the functions of various neurotransmitters in the brain. Nisoxetine, a potent norepinephrine reuptake inhibitor, can potentially be used to study the norepinephrine transporters using PET. In order to label nisoxetine, a precursor must be made through the demethylation of nisoxetine. The precursor will react with [11C]CH3I in order to create [11C]nisoxetine for PET studies. The synthesis of the precursor was attempted using both N-demethylation and O-demethylation techniques. N-demethylation was carried out using the reagent 1-chloroethyl chloroformate while O-demethylation was attempted using a diphenyl phosphine and butyllithium complex. A desired product was obtained in model reactions, however, demethylation of nisoxetine did not afford the desired precursor. These studies provide valuable information in choosing an appropriate protecting group for the amino function before the O-demethylation. Further investigations are underway.

New Methods for Protein Analysis Using Ultra Violet/ Visible Spectroscopy. NGOC-DUNG THANH (*University of Colorado at Boulder, Boulder, CO 80309*) BONNIE HAMES (*National Renewable Energy Laboratory, Golden, CO 89401*).

Some waste biomass is becoming more useful in biomass to ethanol conversion. We are trying to understand the composition of biomass and how it varies naturally. Thus, we need protein analysis to better understand the process that converts biomass into ethanol. The Biofuels Ethanol Program wants to be able to monitor protein content in biomass and track it through ethanol conversion process. Corn stover,

a waste biomass, is used in this analysis. Lignin is one of the substances that give corn stover its structure and it is toxic to all the organisms currently used to ferment sugars to ethanol. And so, we would like to be able to answer, does the presence of protein in the liquid process stream interfere with lignin measurements? Lignin was measured using UV/visible-Spectroscopy. Amino acids, the bases of protein were also measured using UV/visible spectroscopy. Then lignin and amino acids spectrums were compared for interference. Last but not least, a new method for protein analysis was developed.

Characterization of Polymer Electrolytes for Electric Vehicle Batteries. MOSES UKAOMA (Howard University, Washington, DC 20059) JOHN B. KERR (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The lithium polymer battery offers the best option for powering electric vehicles (EV) both now and in the future. The high energy of the lithium metal makes this possible. However, more enhancements are needed to meet the required conductivity of the polymer electrolyte for the application of lithium batteries in EVs. The Department of Energy set a goal of 10^{-3} S/cm for conductivity. In an effort to reach this goal, our research group has developed new polymer architectures and solvation structures to prepare new components that make up the lithium polymer battery. A polyethylene Oxide (PEO) is used as a backbone, and combed side chains attached to it. The individual backbone structure is then cross-linked to one another. In the end, we have a wavy, net-like looking structure (more like steamed spaghetti). While the backbones stay the same, we varied the attached side chains to make different polymers. We chose three different salts, lithium bis(trifluoromethylsulfonyl)imide (LiTFSI), lithium triflate (LiTf), and lithium tetrafluoroborate (LiBF₄), each having unique attributes to match up with our polymers. Combining the salts and polymers gave us different electrolytes, which we tested for T_g (glass transition temperature) and conductivity under various temperatures and concentrations. Our results showed that there is not much difference between the polymers, but significant differences were noticed among the three salts in their various concentrations over the measured temperatures.

Oxidative Leaching of the Hanford Tank Waste using H₂O₂. MELISSA VERHAEGHE (Lewis University, Romeoville, IL 60446) KEN NASH (Argonne National Laboratory, Argonne, IL 60439).

Numerous methods have been proposed to assist in the cleanup of the tank waste that has accumulated at the Hanford site, due to years of production and purification of Plutonium for defense purposes. There are four main types of sludges found at the Hanford site, all of which are simulated in laboratories for further experimenting. They are bismuth phosphate, bismuth phosphate modified, REDOX, and PUREX. The main objective of oxidative leaching is to remove as much Cr, Al, P, and S as possible, without mobilizing trans-uranium elements such as ²³⁸Pu. The research project entailed the use of various concentrations of H₂O₂ and the analyses of the corresponding response of the transition metals. This was accomplished using a Cary-14 Spectrophotometer with an OLIS upgrade package. Results obtained conclude no major significant change in comparison to the two washes used currently at the Hanford site.

Arsenic Removal, Problems, and Solutions with a Special Focus on Third World Countries. KIEM VU (Cosumnes River College, Sacramento, CA 95828) MIKE KAMINSKI (Argonne National Laboratory, Argonne, IL 60439).

Arsenic contamination has become a worldwide epidemic, especially in developing countries where a significant percentage of the population depends on groundwater for drinking. Contaminated groundwater have been found in Argentina, Chile, Mexico, Hungary, West Bengal, Bangladesh, China, Taiwan, and Vietnam. Chronic exposure to arsenic contaminated water at above 50 mg/L can result in serious health problems, such as skin lesions and cancer. The World Health Organization (WHO) current guideline for arsenic in drinking water is 10 mg/L, but all developing countries are still struggling to keep up with 50 mg/L standard. There are many effective arsenic treatments, but unfortunately they are not available to third world countries due to the cost of the technologies. Adsorption and precipitation processes are now being explored for low-cost and effective arsenic removal, which is the focus of this arsenic review. These processes make use of extractants and adsorption medias, such as ferric chloride and iron oxide coated sand to remove arsenic. Most technologies utilizing adsorption and precipitation processes

require an oxidation pretreatment to convert As (III) to As (V) because As (V) adsorbs and reacts more strongly onto the solid phase than As (III). This review also lightly touches on arsenic chemistry and groundwater environments.

Synthesis of Alkyl Carbonate Salts. MATT WEAVER (Shasta College, Redding, CA 96049) JOHN LINEHAN (Pacific Northwest National Laboratory, Richland, WA 99352).

Current industrial processes for carboxylation involve the use of the environmentally toxic chemical phosgene, the use of which produces hydrochloric acid byproduct. Phosgene is widely used in the production of dialkyl and diaryl carbonates, from which products such as polycarbonate resins, fuel additives and solvents are produced. A more environmentally sound compound that has the potential to replace phosgene in these processes is dimethyl carbonate (DMC). It has been deduced that DMC can be produced by reacting CO₂ (which is relatively benign), with an alcohol and a tertiary amine under mild conditions. An intermediate formed in this process is an alkyl carbonate salt. In order to better understand and develop the chemistry of DMC formation, this study examined the formation of several alkyl carbonate salts. The salts were produced using a variety of alcohols, amines, and solvents under varied pressures of CO₂. They were then analyzed by 1H-NMR and 13C-NMR spectroscopy. The study of the production of DMC is ongoing, but preliminary results have provided insight into the amines and solvents that produce the best yields.

Preparation via Self-Assembly of Submicron-sized Silica Bead Monolayers for Surface-Enhanced Raman Scattering. MICHAEL WEAVER (University of Tennessee, Knoxville, TN 37996) SHENG DAI (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Surface-Enhanced Raman Scattering (SERS) allows easier detection of many analytes than typical Raman spectroscopy. For SERS, analytes are usually adsorbed onto metal, primarily silver, atoms. A drawback of this technique is that the silver surface is easily changed, but this vulnerability can be avoided by supporting the silver with a substrate. One substrate, notable for its thermal and temporal stability, is silica beads. In this experiment, a layer of one bead's depth was prepared to observe its performance, once coated with silver, as a SERS substrate. Several populations of monodisperse silica particles were prepared using the Stöber synthesis. In some cases, the hydrophilic surface of the beads was modified to be more hydrophobic by binding alkyl groups to the surface; this modification was done in order to effect the self-assembly of small (400nm) beads. The beads were then dispersed in organic solvent and ethanol to form a colloid. This colloid was lowered onto an aqueous phase, and the repulsion between the water and the organic solvent surrounding the beads provided force for self-assembly of a silica bead monolayer. This monolayer was applied to both glass and silicon substrates. Scanning electron microscopy (SEM) was used to evaluate the homogeneity of the monolayers generated. For bead diameter sizes of approximately 800nm and 400nm, a homogeneous monolayer was successfully and consistently produced. Early testing of this monolayer substrate for use with SERS indicates a lower relative standard deviation (RSD) of results than with multilayer silica substrates. These preliminary results suggest SERS may improve as a quantitatively useful tool.

Purification of Single-Walled Carbon Nanotubes. BRIANNA WHITE (Saginaw Valley State University, University Center, MI 48710) PHILLIP BRITT (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Single-walled carbon nanotubes have generated a lot of interest in the scientific community because their remarkable properties could lead to many useful applications. In order to develop these applications, the carbonaceous impurities and metal catalyst that form on the tubes when they are made must be removed. The standard purification procedure at ORNL involves refluxing the tubes for 17.5 hours in 3M HNO₃, filtering, thermally oxidizing at 450°C, sonicating in HCl, thermally oxidizing at 500°C, and sonicating again in HCl. This procedure only results in 6-10% yield of tubes with less than 1 weight percent metal. The goal of this research is to improve the yield and purity of the tubes. The reflux time, acid molarity, method of physical separation, and chemical oxidizing method were varied to achieve this. Each variation was characterized by SEM, TG-MS, and TGA. The tubes were refluxed for 8, 16, 32, and 64 hours and it was found that increasing reflux time results in a lower yield of tubes containing more metal impurities. The molar concentration of nitric acid was increased to 6M, but no difference in yield or quality was observed from the

sample that was refluxed in 3M HNO₃. A standard sample was split in half and one part was centrifuged while the other was filtered. The SEM images as well as the TGA traces indicate that the centrifuged sample contains more impurities. 20% H₂O₂ was used as the chemical oxidizing reagent and the SEM and % yield results were encouraging. Further investigation of this method will be preformed.

Metastable Beam Source via Two Photon Pumping Technique.

WILLIE WONG (Princeton University, Princeton, NJ 08544) **LINDA YOUNG** (Argonne National Laboratory, Argonne, IL 60439). Metastable beams of rare gas atoms have wide applications in chemical analysis of samples, as well as in aiding understanding of fundamental processes and physical attributes. Most current sources of metastable rare gas atomic beams, however, are limited in their flux density, and thus greatly reduce their application in applications such as low level trace analysis and precision measurements. Previous work has demonstrated feasibility of metastable krypton production via two-photon pumping, and this paper extends that possibility into beam form. Further optimization on this scheme, moreover, promises 100-fold increase of metastable krypton flux density over that of an rf-driven discharge.

Preparation and Characterization of Electrodes for Use in Proton Exchange Membrane Fuel Cells.

JOHN YI (Princeton University, Princeton, NJ 08544) **ANDREW BOCARSLY** (Princeton Plasma Physics Laboratory, Princeton, NJ 08543).

A major problem associated with many current energy systems is their negative environmental impacts. Therefore, research into alternative forms of energy is crucial. Hydrogen fuel cells are one possibility, as they produce no pollution; water and heat are the only by-products. The particular type of fuel cell examined was the polymer electrolyte membrane (PEM) fuel cell, also known as the proton exchange membrane fuel cell. Membrane-electrode assemblies (MEAs) were constructed using electrodes prepared by two different techniques. In one method, the electrocatalyst active layer was pipetted onto the electrode directly, while in the other method the catalyst was air-brushed onto the electrode. The electrocatalyst employed included carbon-supported platinum and various carbon-supported platinum alloys (Pt/Cr, Pt/Co). The MEAs were characterized by evaluating their performance on a fuel cell test station. The reactant gas temperatures, cell temperature, flow rate, gas pressure, and humidification conditions in the fuel cell were varied in order to generate current-potential curves. This allowed for an investigation into the possibilities for the best carbon-supported platinum alloy electrocatalyst for the oxygen reduction reaction in the fuel cell.

Optimizing Electrodes for Rechargeable Batteries.

JENNIFER YOUNKER (University of Louisville, Louisville, KY 40292) **ARTHUR KAHAIAN** (Argonne National Laboratory, Argonne, IL 60439). The goal of the research was to explore new and existing rechargeable battery electrodes. One of the experiments involved cycling lithium battery cells in which the spinel powder in the cathode was coated with either aluminum oxide or zirconium oxide. The coating inhibited the degradation of the spinel in the battery cathode, which is normally seen in the uncoated cells when cycled over time at elevated temperatures. Layered electrodes were also examined. The experiment performed on the layered cathodes was an attempt to synthesize xLiMn_{0.5}Ni_{0.5}O₂ × (1-x)Li₂TiO₃ using TiO₂ powder instead of Ti[OCH(CH₃)₂]₄ solution, since the solution samples are difficult to measure. The solid TiO₂ powder was successfully used in the synthesis, and is preferred for industrial application and synthesis. A third electrode experiment involved testing magnesium anodes in a rechargeable battery. The cells cycled successfully and a voltage window of 1.7 to 1.2 volts was discovered for the magnesium/V₂O₅ cell.

COMPUTER SCIENCE

Perform Genomic DNA Assembly and Annotation at National Energy Research Scientific Computing Center (NERSC), LBNL. **JENNY YJ CHUU** (Las Positas, Livermore, CA 94550) **JONATHAN CARTER** (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

To implement IBM supercomputer at NERSC to be a robust, scaleable platform to contribute to the Bioinformatics research communities is the goal of this research work. The strategies are to integrate user data sources, data mining, and visualization tools into a single framework

without the need to display any of the complicate hardware and software systems. The analysis tools are responsible for the diverse data mining to facilitate the building of complex data analysis pipelines. The outputs of these tools can be chained into an analysis protocol and thus facilitates high throughput analysis. In this study, we emphasize to implement and automate of analysis tools. BLAST, phrap, phrapview, and formatdb software and mouse whole genome shotgun DNA sequences and Univect databases are installed. Perl and shell scripts are used to automate the file processes. The results presented in this paper have successful demonstrated DNA sequence assembly and annotation by using installed tools, databases, and scripts in the IBM supercomputer at NERSC.

Hemoglobin Subgroup Classification Using Parallel Supervised Computer Learning. **RYAN CUNNINGHAM** (University of Cincinnati, Cincinnati, OH 45039) **RICHARD VILIM** (Argonne National Laboratory, Argonne, IL 60439).

We classified hemoglobin proteins by subgroup using agglomerative cluster analysis. The distance metric for the cluster analysis was a novel, weighted similarity matrix generated by a genetic algorithm implemented on a parallel PC cluster. The genetic algorithm used a supervised learning strategy. Its fitness score compared each member of the population's clustering against the true subgroup classification. Once an optimum solution was found for the training data, the solution was run with test data to verify its generality.

A Survey of Registration and Segmentation Methods. **SARAH OSENTOSKI** (University of Nebraska, Lincoln, Lincoln, NE 68588)

MIKE PAPKA (Argonne National Laboratory, Argonne, IL 60439). Scientific visualization allows scientists to view their data in meaningful context. In the case of medical visualization, where the human body is the subject, it is more intuitive for scientists to visualize the body in a three dimensional view. Our project focuses a survey of five segmentation and registration methods being used to perform analysis on medical images. The methods we will review are watershed segmentation, snake segmentation, and morphogenesis. The registration methods are anatomical landmark registration and registration using mutual information. A brief overview of each method is given. The feasibility and effectiveness of each method is also discussed.

XML Structuring of Airflow and Pollutant Transport Simulation Input Data. **WILLIAM WATTS** (City College of San Francisco, San Francisco, CA 94112) **DAVID LORENZETTI** (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

Anth-Trax is a pollutant transport modeling program that predicts the spread of anthrax spores and other aerosol particles within a building. Spores can spread through advection in airflows, deposition to room surfaces, and resuspension and tracking due to human activity. The model tracks the resulting accumulation of spores in air, and on floors, walls, filters, and ventilation ducts. Predictions made by the model can help answer questions about the transport and fate of aerosols in a building. The existing program uses cluttered, unstructured input files. This forces users to expend an undue amount of effort writing and verifying input, rather than interpreting simulation results. This project used XML to provide a structured interface to the program. XML is a markup language, similar to HTML, that supports user-defined formats for identifying data. We integrated an open-source XML parser into the simulation program. The parser reads an XML input file, checks that it obeys basic structural rules, and passes the data to Anth-Trax. This required defining a set of XML tags to express the simulation data, and rewriting the Anth-Trax input routines to accept XML. The new input files are easier to create, and the existence of free software for displaying and manipulating XML helps non-experts understand the structure and meaning of a simulation. Finally, the use of XML should aid the implementation of a graphical user interface for Anth-Trax.

Programming a Spreadsheet Application in Microsoft Excel using Visual Basic for Applications (VBA) for The Proton Transfer Reaction Mass Spectrometer (PTR-MS). **LUIS ACEVES** (Southwestern Community College, Chula Vista, CA 91910) **MICHAEL L. ALEXANDER** (Pacific Northwest National Laboratory, Richland, WA 99352).

The PTR-MS provides real-time volatile organic compound (VOC) data that can be correlated with chemical and meteorological data. These measurements aid in developing computational atmospheric chemistry models that predict urban ozone and particulate levels. The data is stored in a binary data format by the mass spectrometer, the data must

be converted to an ASCII file using a software application called Balzers, then this file must be imported into Microsoft Excel so that the data can be analyzed. Upon importation, the data is formatted to an understandable presented database in Excel. The process of formatting is very tedious, time consuming and involves many keystrokes and changes to the file. Creating this program using VBA will perform all the necessary formatting with the click of a button in the toolbar, saving time and preventing errors. This will make the analysis of such data easy to generate graphs and charts for future presentations of experiments to come.

Super Computing on the Playstation 2. MARK AEVERMANN (Lehigh University, Bethlehem, PA 18015) MIKE PAPKA (Argonne National Laboratory, Argonne, IL 60439).

Computational sciences have grown tremendously in recent years and as this field expands it demands faster and faster computers. These faster machines cost exponentially more than computers used around the home and office, so there is a shortage of cheap high performance scientific computers. One relatively unexplored area of computers capable of doing this high performance computing is that of the console gaming systems. Increasingly the latest generations of console systems have become more like computers, with hard drives, network cards, and support for various programming languages. The latest generations of Playstation console systems have recently developed a kit containing those three key components along with a custom Linux build effectively turning the Playstation 2 (PS2) into a computer. With recent price drops in the cost of the PS2 these systems now appear to have even larger potential for use in the scientific computing community.

A Web Accessible Implementation of the International Commission on Radiological Protection (ICRP) Pub 66 Lung Deposition Model. LIN AHMAD (University of Houston-Downtown, Houston, TX 77002) RICHARD C. WARD (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The International Commission on Radiological Protection (ICRP) publishes a series of reports describing the deposition of airborne radionuclides in the respiratory tract of workers for the purpose of calculating radiation exposure and setting limits for exposures. One of the ICRP reports, Publication 66, sets forth a Lung Deposition Model for deriving percentages of radioactive material deposited in different regions of the lungs based on physiological and environmental factors. Examples of physiological factors include the tidal volume and fractional residual capacity of the lungs; and examples of environmental factors include the wind speed, shape and diameter of the aerosol. This web implementation of the Lung Deposition Model will provide easy availability to the model via the World Wide Web for researchers. Presently, while standalone implementations of the Lung Deposition Model exist, to our knowledge no web-accessible version exists. For this implementation, a Perl script is created to capture input from a web page and execute a standalone C++ implementation of the ICRP Pub 66 model. Results of deposition in regions of the lungs are displayed to the web browser using a Perl script. Extensive documentation of the Lung Deposition Model is provided. This documentation is created using new XML-based paradigms including MathML and SVG (scalable vector graphics) which is used to provide a graphical image of the compartment model. The result is an implementation of a web-accessible Lung Deposition Model that will improve its use by the radiation protection community and introduce this model to the wider physiological modeling community.

The Visual Simulation of a DC Breakdown. ERIK AVER (Montana State University, Bozeman, MT 59715) ANDREW POST-ZWICKER (Princeton Plasma Physics Laboratory, Princeton, NJ 08543).

The computerized visualization of a DC breakdown plasma simulation is a new tool in the exploration of plasma behavior. By modularly building off an existing plasma simulation code, a highly simplified, user-friendly interface is constructed that allows for easy experimentation. The graphical output allows for immediate interpretation just as in the laboratory. Development focuses on running the breakdown simulation, converting the resulting collision effects into atomic emissions, and finally displaying those results by using the actual appropriate color. The atomic physics section uses the electron density and energy calculated by the breakdown simulation to determine the steady-state excitation level populations from which the emission rates for each line are determined for use in visualization. The final simulation package will demonstrate the effectiveness of

modeling and will provide greater access to the concepts of plasma physics.

Improving Web Site Efficiency. JAMES BASCO (Illinois State University, Normal, IL 60515) JACKIE COPPLE (Argonne National Laboratory, Argonne, IL 60439).

The Internet has become an invaluable tool in many aspects of every day life. Although such a powerful media is within the public domain and available for anyone to use, in most situations the idea of creating a web page can be intimidating and difficult. With this in mind, it has been my objective to redesign the public Internet pages for the Chemical Technology Division. The new layout that has been implemented uses several techniques to create a template that can be used by anyone with minimal knowledge of computers and the Internet. By creating the template we have allowed people within the division to create their own pages by simply inserting the body of the document. In the process we have also employed the use of other techniques that will allow us to change the format of every page within the web site by altering a single file.

Design and Implementation of a Data Analysis/Monitoring Computational Engine. DAVID BAUER (Georgia Institute of Technology, Atlanta, GA 30332) GEORGE OSTROUCHOV (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Scientific simulations (e.g., climate modeling and supernova explosion) typically run for at least one month and produce data sets in the order of one to ten terabytes per simulation. These numbers are expected to continue to grow. The ability to analyze this data in an effective and efficient manner is critical for both scientific discoveries and the utilization of human and computing resources. Current generic analysis tools must either wait until the simulation is finished, or interfere with the running simulation simply to access the data. They are then faced with hardware and algorithmic limitations native to the huge data sets. Tools written to deal with these limitations are often application specific. The DOE Scientific Data Management Integrated Software Infrastructure Center (SDM-ISIC) has been developing an Adaptable Simulation Product Exploration and Control Toolkit (ASPECT) that will enable effective and efficient monitoring of data generated by long running simulations ("run and render" framework) through the GUI-based interface to a rich set of pluggable data analysis modules. The design that evolved integrates the open source R statistical data analysis package, as a general computational back end, with a controller that directly understands the commonly used NetCDF file format. By using R scripts and XML function descriptions, users can easily and quickly add specialized functions and macros to the already comprehensive R libraries available. With the shortly expected integration of (already written) data complexity reduction routines (dimension reduction and clustering), the generic or specific analysis of very large data sets can be accomplished.

Multi-modal Data Visualization Component Research.

MICHELLE BEGAY (Arizona State University, Tempe, AZ 85287) RYAN E. HOHIMER (Pacific Northwest National Laboratory, Richland, WA 99352).

The problem involved getting instruction from my mentor Ryan E. Hohimer. In order to pursue further experiments, Environmental Molecular Sciences Laboratory (EMSL) needed assistance from and collaboration with the Information, Science and Engineering (IS&E) department. My participation in the project was to program a graphical user interface. I undertook the problem using four methods: Analyze, Design, Implement, and Test. The results of the project are implementations of object-oriented programming. I discovered using the four suggested methods and implementing the graphical user interface was a task worthwhile. The effort to learn object-oriented programming is continuous. The graphical user interface produced is a prototype and will result in future re-structural phases.

Network Resource Database (NRD). DON BIBLE (Mississippi State Technical Community College, Knoxville, TN 37933) TERRY HEATHERLY (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Computing and networking resources are depreciatory cost elements for most business organizations. Within the Engineering and Science Technology Division (ESTD) at Oak Ridge National Laboratory, a recent review of the Network Resource Database (NRD) suggests that ESTD employees are utilizing approximately 1100 data network connections to support their diverse research activities, at an annual operational expenditure of \$425K. The NRD, in conjunction with the SAP business

system, was used to develop a database specific to ESTD's operational expenses for networking support services. The NRD provided data for each staff member's usage and the number of responsible network resources. SAP provided organizational information (e.g., employee's name, an organizational id unit, etc.). Preliminary analysis suggests that numerous active network devices could potentially be eliminated, resulting in a reduction in operational expenditures. Quantitative analyses of the developed database will be performed with the objective of reducing unnecessary recurring costs.

Creation of the Pipeline Graphical User Interface(GUI). KELLY BIRCH (*Utah State University, Logan, UT 84322*) PAUL D. ADAMS (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The complete automation of the x-ray crystallographic process is necessary in order for high throughput structural genomics to be practical. The Pipeline project at beamline 5.0.3 of the Advanced Light Source is automating the x-ray diffraction experiment and data processing (integration and scaling). The collected data resides in a digital world and is accessible only through a user interface. Currently the most common method for human interaction with this type of information is a graphical user interface (GUI). Creation of a simple, intuitive graphical user interface empowers scientists to quickly ascertain the results of the experiment and the validity of those results. To mitigate the learning curve of this software, the graphical user interface utilizes the conventions of other similar software in existing x-ray crystallographic software programs. This software is implemented with a platform-independent, python-based language, i.e., wxPython. The data for the experimental results and the data processing are stored on different computers; therefore, the GUI is part of the distributed computing environment. Alexander Birch has created this graphical user interface.

The Geometries of the ATLAS Experiment. NATHAN BOWER (*Rochester Institute of Technology, Rochester, NY 14623-5603*) KEITH LALLY (*Brookhaven National Laboratory, Upton, NY 11973*).

The use of data analysis software, like ROOT, for observing theoretical high energy physics data is important in the studies of theoretical large hadron collisions inside of particle colliders, such as the ATLAS collider that's being constructed in Geneva, Switzerland. Incorporating the ability to design particle collider geometric shapes (tube, cube, etc...) in this software is another key element in the studies of the theoretical collision data. Using the attributes to define volume and position in ROOT, to help define the same attributes in another software program designed for data visualization is another key part of the research. The importance of this file conversion becomes apparent when a researcher can see the actual shape of a particle detector with the theoretical event data inside of it. Possessing the ability to extract certain sections of the data and analyzing the removed section independent of the main detector is a main goal of our project.

Development of an Interactive Code for the Calculations of Radionuclide Production in a Nuclear Reactor. ABBIE BRANNON (*Wesleyan College, Macon, GA 31210*) SAED MIRZADEH (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Over the past decade, a computer code, LAURA, has been developed and used by a limited number of researchers to determine the production of isotopes in a nuclear reactor. This code is written in Fortran and runs in DOS. The LAURA user must have at least some knowledge of Fortran and DOS to run the program. However, by incorporating the Fortran code into a Visual Basic developer, the code takes on the form of a windows environment making the program more accessible to the average user. The user is given a visual representation of the nuclides chart and the choice of selecting target and product nuclei, and options on irradiation time, neutron flux, etc. The Visual Basic code does not yet incorporate all the radioactive decay or neutron transmutation options that were incorporated in the original LAURA. Over time, these will be programmed in along with more user options. When fully developed, the interactive LAURA will be a useful tool for the calculations of radionuclide production in a nuclear reactor.

The Genetic Algorithm as a Means of Modeling Electrical Power Buying Patterns. JENNIFER CAMP (*Southwest Baptist University, Bolivar, MO 65613*) VICKIE E. LYNCH (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Computer simulations to predict the cost of electricity could be very helpful as the power industry is further deregulated. To most accu-

rately reflect the buying practices of utility companies, the simulation must employ a form of artificial intelligence in order for the utilities to learn the most effective bidding strategies. The genetic algorithm was used to simulate the learning techniques of the utilities, which were represented as intelligent agent objects. The agent's bids were calculated using a set of predetermined rules, and each chromosome of the genetic algorithm represented what rules the agent was currently utilizing. After each bid, these chromosomes were manipulated using the standard reproduction, crossover, and mutation procedures of the genetic algorithm. According to the principles of self-organized criticality, one would expect the total of the agent's bids to organize near the critical point, which is the total amount of electricity available. The final version of the simulation showed evidence that the agents were learning and that the bids were organizing to a value near the critical point. Closer examination revealed that the agents were often converging to one or two sets of rules, and retained those rules until a mutation occurred. Occasionally an agent would converge to a very poor set of rules that would produce very low or very high bids. The use of genetic programming is currently being researched in an attempt to eliminate this problem of early convergence.

Rectangular Cell Substrate Impedance Model. ROBERTSON CAMPBELL (*Southwest Baptist University, Bolivar, MO 65613*) RICHARD WARD (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Computer simulations are a resourceful tool for analyzing data from scientific experiments. For a layer of cells on a gold electrode, numerical simulations of the electrical potential between the cells and electrode can be used to estimate important physical properties of the cell. The sub-cellular potential, V , can be described by the two-dimensional complex Helmholtz equation in rectangular coordinates, estimated using a five-point finite difference (FD) approximation. A block cyclic reduction direct matrix solver from the FISHPACK FORTRAN library was used to solve the resulting block tri-diagonal complex matrix equation. The numerical solution of V agrees with the analytical solution for a constant Dirichlet boundary condition, although the analytical solution was difficult to compute accurately. The FORTRAN subroutine, DAVINT, was used to integrate V and the result was used to compute the total impedance of the cell-covered electrode, Z_c . The numerical estimated Z_c agrees with the analytical Z_c for the corresponding one-dimensional radial problem. A user-friendly graphical user interface (GUI) was designed to perform parameter sensitivity analyses, initially for frequency only. The GUI incorporates the Compaq Array Viewer for displaying three-dimensional graphs of the real, imaginary, and magnitude values of V and two-dimensional graphs of Z_c as a function of frequency. Interfacing the GUI to the numerical simulation required linking C++ and FORTRAN routines.

Implementing the Cyber Security Program Plan for the Facilities and Operation. EDGARDO CARASIG (*State University of New York at Stony Brook, Stony Brook, NY 11790*) PATRICIA WILL-IAMS (*Brookhaven National Laboratory, Upton, NY 11973*).

Cyber Security is a serious issue at Brookhaven National Laboratory (BNL). Thousands of cyber attacks a day are recorded in the Intrusion Detection System (IDS) and it is important that the BNL network is secure. BNL and the Department of Energy (DOE) have worked together to develop a Cyber Security Program Plan (CSPP) that will lead to a more efficient and more secure network. The assignment I have been given entails implementing the CSPP for all of the Facilities and Operations Directorate. This division alone consists of approximately 300 personal computers as well as about 550 users. Each computer must be prepared to accommodate Cyber Security Patches. These are the files downloaded into the computer that detect if the unit is being infiltrated. Next, a scanning application is installed for determining if all Operating System and Internet Explorer patches have been installed. This program also makes it easier for users and System Administrators to determine if they need any further patching in the future. If an instance occurs where an individual or group is attempting to utilize the tools and resources of the division by accessing secure information then a report is made at IDS.

Addressing Noncontiguous I/O Access Through MPI-IO. AVERY CHING (*Northwestern University, Evanston, IL 60201*) ROBERT ROSS (*Argonne National Laboratory, Argonne, IL 60439*).

The message passing programming model is the dominant model for

parallel programming today, mainly due to availability of implementations of the MPI 1.2 specification on the majority of platforms. Today we see more wide spread use of MPI software among developers and users. MPI has also gained acceptance as a high-performance portable platform to build upon by higher level APIs. The addition of the MPI-IO features has allowed for many optimization opportunities over the traditional POSIX interface. In order for MPI-IO to utilize this opportunity, underlying file systems must provide such capabilities. Multiple studies have found noncontiguous I/O a large bottleneck in many scientific applications. A method of reducing the large overhead of noncontiguous I/O involves creating the capability for MPI-IO to understand noncontiguous I/O calls natively and passing this description on to an underlying file system that can make use of such a complex description. The Parallel Virtual File System (PVFS) has the ability to understand the list I/O interface and process it effectively. We have augmented ROMIO, the MPI-IO implementation at Argonne National Labs, to utilize PVFS's list I/O interface as an optimization for noncontiguous data access. In this paper, we present the list I/O interface for ROMIO using PVFS. We show the results of several noncontiguous data access benchmarks and discuss the future of further optimized noncontiguous data access.

Graphical Display of Sensory Feedback. ZANE CHRANE (*North Carolina State University, Raleigh, NC 27607*) TOM EWING (*Argonne National Laboratory, Argonne, IL 60439*).

Current visualization systems used in telebotanic manipulation are very limited in their capacity to allow operators to safely and efficiently decommission and decontaminate materials used in contaminated environments. These limitations stem from the fact that current systems normally only consist of two dimensional television displays that lack elements of depth perception and non-visible information such as force vectors, stress, strain, etc.. The purpose of my research has been to develop computer generated graphical representations of these types of information to be superimposed onto a stereo video system display. Using various sensors in the remote environment, we are able to input the information via serial ports to be displayed both graphically and numerically as part of the display system. These developments provide many benefits to the operators in both safety and efficiency of operating the remote manipulators.

Improving the Security of SCADA System Data Transmission. TYLER CHUBB (*University of Wyoming, Laramie, WY 8070*) JEFFREY M. JOHNSON (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The electric power transmission infrastructure of the United States is becoming increasingly reliant on supervisory control and data acquisition (SCADA) systems for control and monitoring purposes. Computers in centralized locations are rapidly replacing operators manually controlling equipment and recording data. The security of SCADA system communications is understandably of significant importance to our nations national security. It was shown in earlier phases of this project that since many SCADA protocols contain little to no provision for message encryption and authentication, it is often easy for an infiltrator who has gained access to a communications channel to send fraudulent control commands to automated equipment, which could potentially disable power transmission to a wide area. The overall long-term project goal is to improve the security of SCADA systems by incorporating authentication into messages exchanged between SCADA system components. An immediate project goal involves constructing custom-built software that implements the Distributed Network Protocol (DNP), a protocol widely used for transmitting data in modern SCADA systems. Having this custom-built DNP software will be advantageous, as it will allow modifications to the DNP protocol at levels necessary to experiment with security enhancement.

Optimization of Functions using Genetic Algorithms. SCOTT CLARK (*University of Tennessee, Knoxville, TN 37996*) JUAN FERRADA (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*). Optimization is a useful mathematical technique for finding a maximum or minimum value of a function. In today's factories, achieving the maximum production at the minimum cost is the ideal manufacturing philosophy. For years, chemical engineers have sought after better ways to design and operate plants. By applying computer simulation, an inexpensive and resourceful way to predict outcomes, these engineers can reduce safety risks while manipulating specific features, i.e. pipe diameters, of chemical waste disposal facilities.

Software that develops chemical flow sheets (FLOW), as well as a program that performs Genetic Algorithm calculations (LGADOS) was linked by an object-oriented interface (GNTST) to allow FLOW to employ LGADOS resources. The LGADOS program was modified to take a random array of pipe diameters and calculate the costs of using each diameter of pipe. A Genetic Algorithm equation was utilized in the LGADOS program to achieve a parabolic curve, from which the minimum cost could be derived. GNTST was then used to generate an output consisting of a pipe diameter size that is dependent on the minimum cost necessary to achieve the maximum production. As a result, FLOW and LGADOS are able to communicate because of GNTST, and generate the most cost efficient, productive pipe diameter size for use in Chemical Waste Disposal Facilities.

Mathematical Analysis of Oscillatory Metabolic Networks. DAVID DEHORN (*Northwestern University, Evanston, IL 60201*) MICHAEL MINKOFF (*Argonne National Laboratory, Argonne, IL 60439*).

The mathematical models of cellular regulation, specifically of the activity of certain substrate-enzyme complexes, are understandably of paramount importance to those who wish to understand the intricacies of cellular action. Using modern turnkey packages, particularly MAPLE 8 and MATLAB 6, guided explorations of parameter spaces and bifurcation analysis produced much insight into several abstractions governing cellular oscillatory behaviors. Using these modern packages to explore historical papers, as well as perform unprecedented mathematical analyses, helped to introduce many simplifications to existing models and attain further insight into the mathematics governing cellular self-oscillations with, and in the absence of, various feedback mechanisms. An exploration into equilibrium continuation using an external MATLAB package is currently being undertaken in an effort to produce supplementary understanding.

Supporting Grid Computing with Java. IGOR DINER (*Pace University, New York, NY 10038*) GREGOR VON LASZEWSKI (*Argonne National Laboratory, Argonne, IL 60439*).

The notion of Grid computing is best explained in practice by referring to the Globus Project, which attempts to provide the scientific community with 'integrated, collaborative use of high-end computers, networks, databases, and scientific instruments'. An important goal of Grid research has been the introduction of frameworks that utilize popular commodity technologies for interaction with the Globus Services. The Java Commodity Grid (CoG) Kit provides a user-friendly approach to Grid computing. Java is easy to learn and popular in undergraduate curriculums, making the Java CoG Kit an ideal tool for introduction of undergraduate students to the Grid community. Expanding this framework and making it further accessible for undergraduates is a task best suited for undergraduates themselves. As newcomers to the Grid community we have come across problems and setbacks that an expert user might overlook. Utilizing our unique perspective on the subject at hand, we have endeavored to simplify common tasks such as the installation of the Java CoG Kit. Furthermore, we strive to expand the documentation and information portals as well as to develop sample programs that showcase the easy use of Grid technologies, hoping to flatten the learning curve and promote a deeper involvement of Grid computing with Java.

Evaluation of the Open Source Program Vis5D. AARON FISH (*Jamestown Community College, Jamestown, NY 14701*) CARMEN BENKOVITZ (*Brookhaven National Laboratory, Upton, NY 11973*). Today there are numerous software packages that enable the visualization of data. Finding the right package is time consuming and difficult. The user's computer experience, the type of data to be represented, and the amount of time a user needs to learn a new software package are among the more important matters to evaluate. For the visualization of aerosols in the Earth's atmosphere the open-source program Vis5D was chosen. Dr. Carmen Benkovitz is studying the magnitude of the perturbation of the Earth's radiation balance caused by atmospheric aerosol. Carmen provided model output (moput), part of a 6-week simulation of the Northern Hemisphere. Vis5D is an efficient tool that allows visualization of large, complex multidimensional data sets. For Carmen's application, the variables to be studied needed a four-dimensional charting of latitude, longitude, altitude, and time. This is the reason organizations such as the EPA and the National Weather Service also use the Vis5D program. Vis5D is open-source software and therefore comes with no guarantee and

very little technical support. For users that have little or no computer experience the downloading and installation of Vis5D can be a daunting task. Vis5D uses a trivial amount of meteorological terminology and therefore a general knowledge of meteorology is also beneficial. Any data that are imported to Vis5D must be in a .v5d format.

Data Resources of the Recharge System. *KEREN FU (Bunker Hill Community College, Boston, MA 02129) CHARLES E. VERBOOM (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).* Information technology is one of the significant roles in today's dynamic business industry. In the field of information systems development, five systems development life cycle (SDLC) phases have been defined: systems planning, systems analysis, systems design, systems implementation, and systems operation and support. Among these phases, systems analysis is the specific one being utilized on an internal recharge system in Lawrence Berkeley National Laboratory. System Analysis is a phase for people to understand data process within an information system and build a logical model of it. Techniques those are used in this project include Requirements Modeling, Data Modeling, Process Modeling and Object Modeling. After documentation and analysis, there are several potential improvement opportunities identified, such as user validation, backup system and potential coding redundancy, etc. Feedback and suggestions were provided to the system maintenance programmers.

Using WIRED to Study Simulated Linear Collider Events. *AYANAH GEORGE (Bethune-Cookman College, Daytona Beach, FL 32114) TONY JOHNSON (Stanford Linear Accelerator Center, Stanford, CA 94025).* The purpose of this project is to enhance the properties of the LCD WIRED Event Display. By extending the functionality of the display, physicists will be able to view events with more detail and interpret data faster. Poor characteristics associated with WIRED can severely affect the way we understand events, but by bringing attention to specific attributes we open doors to new ideas. Events displayed inside of the LCD have many different properties; this is why scientists need to be able to distinguish data using a plethora of symbols and other graphics. This paper will explain how we can view events differently using clustering and displaying results with track finding. Different source codes extracted from HEP libraries will be analyzed and tested to see which codes display the information needed. It is clear that, through these changes certain aspects of WIRED will be recognized more often allowing good event display which lead to better physics results.

Scientific Visualization on High Resolution Flat Panels. *BRIAN GRINNELL (Alfred State College, Alfred, NY 14802) MICHAEL MCGUIGAN (Brookhaven National Laboratory, Upton, NY 11973).* The goal of this project was to implement visualization tools with a high-resolution flat panel display. The display that was used in this project was an IBM T221 22.2 inch LCD display that has over 9.2 mega-pixels. This display is being driven by an IBM intelligistation with a Windows 2000 operating system. There were three visualization tools to be evaluated on this display: OpenDX, VolView, and Amira. To help evaluate these programs, data sets from computer microtomography, weather, and medical were used to see how applicable each program was to the particular data.

Techniques of Testing and Debugging. *LUCA HALL (Community College of Rhode Island, Warwick, RI 02842) JONATHAN TAYLOR (Brookhaven National Laboratory, Upton, NY 11973).* Debugging is what programmers do when they know that a program is not working correctly. Testing on the other hand is a determined, systematic attempt to break a program that the programmer thinks is working. This paper will focus on techniques to find errors rapidly and effectively. Thinking about potential problems as you code and while you code is a good place to start. Systematic testing and debugging from simple to complex tests will help to ensure that programs begin by working correctly and remain correct as they grow.

Development of Ladder Logic Code for SNS Beam Dumps using the Programmable Logic Controller. *BRIGITTE HSEUH (Johns Hopkins University, Baltimore, MD 21218) BRIAN OERTER (Brookhaven National Laboratory, Upton, NY 11973).* The use of neutrons in experimentation is currently widespread, due to

their superior probing capabilities. However, the most efficient method of neutron production, by a nuclear reactor, is potentially dangerous to both people and the environment. The SNS project employs a process known as spallation, where atoms eject neutrons from their nuclei. A high-energy beam of protons is directed towards a liquid mercury target, from which the neutrons come. Two beam dumps are provided in the SNS facility. The first, at the end of the HEFT end of the LINAC permits tuning up the LINAC when the ring is not available. The second is between the ring and target to allow testing of the apparatus without sending the beam to the target. The beam dumps are large blocks of absorbing material. However, due to the high amount of energy in the beam, the temperature of the dump can rise to 600 degrees or higher. An array of twenty-eight thermocouples along with an Allen-Bradley PLC was chosen to monitor these temperatures. The thermocouples are connected directly to the PLC through specialized modules. A GUI developed with the EPICS system provided a configurable alarm temperature for each thermocouple, as well as control over which thermocouples to be included in the MPS. This was compiled and run through ladder logic code created by the RSLogix5000 software. If any thermocouple were to exceed its given threshold, an alarm signal would be generated for the MPS, resulting in the halting of the beam.

Using Vis5d+ to Visualize Five Dimensional Data Sets on a Three Dimensional Grid. *RONALD HUEGEL (Alfred State College, Alfred, NY 14802) CARMEN BENKOVITZ (Brookhaven National Laboratory, Upton, NY 11973).* The National Weather Service has been using Vis5D to visualize various weather variables such as humidity, wind vectors, and cloud formations for the past several years. Models of atmospheric aerosols have been developed to calculate mixing ratios of SO₄ and SO₂. Two dimensional visualization software tools such as PV-Wave have been used to view the data from these models. In order for today's scientists to better view five dimensional data (longitude, latitude, height, time, and physical variables) on a 3 dimensional grid it is necessary to use more sophisticated visualization software tools. Since meteorological data is similar enough to the data produced by the "MOPUT" (model output) used in mapping atmospheric aerosols we felt Vis5D would be a good candidate for data visualization. We explored/ tested the different versions of Vis5D to determine which one is best for our data and computing platform. We found that earlier versions may work better with certain systems although lacking in some of the features available in later versions (stereo mode, and a function for creating VRML files). Vis5D+ is the most recent version it; however, some of its features are not compatible with SGI machines on which we are running the visualization experiments. Despite some technical difficulties, Vis5D has proved to be a flexible and powerful tool for visualizing MOPUT data.

PC Deskside Support. *ANTHONY IGBOKWE (New York Institute of Technology, New York, NY 10023) MIKE STANGEL (Brookhaven National Laboratory, Upton, NY 11973).* Today, with computer or network related applications pervading more and more of our lives at work and at home, good support infrastructure has become a major factor in many organizations. Computers break and have problems as it is being used during a period of time, one way or the other there is a need support and maintenance services. The PC Deskside support group in BNL provides PC hardware and software support for thousands of its end-users. Many approaches are used to solving computer mishaps. They include defining users computing requirements, specifying appropriate computer hardware and software, identifying sources for equipment and software, ordering necessary materials, receiving and staging computer hardware and software, and installing PC hardware and software and configuring it as required.

Exploring the Use of a Reliable IP Multicast Protocol to Distribute BaBar's Online Event Processing and Filter Software to a Large number of Farm Machines. *TOMOKO ISHIHARA (Reed College, Portland, OR 97202) STEFFEN LUITZ (Stanford Linear Accelerator Center, Stanford, CA 94025).* Currently, the problem at hand is in distributing identical copies of OEP and filter software to a large number of farm nodes. One of the common methods used to transfer these softwares is through unicast. Since the sending rate is limited, this process poses to be a bottleneck. Therefore, one possible solution to this problem lies in creating a

reliable multicast protocol. A specific type of multicast protocol is the Bulk Multicast Protocol [4]. This system consists of one sender distributing data to many receivers. The sender delivers data at a given rate of data packets. In response to that, the receiver replies to the sender with a status packet which contains information about the packet loss in terms of Negative Acknowledgment. The probability of the status packet sent back to the sender is $1/N$, where N is the number of receivers. The protocol is designed to have approximately 1 status packet for each data packet sent. In this project, we were able to show that the time taken for the complete transfer of a file to multiple receivers was about 12 times faster with multicast than by the use of unicast. The implementation of this experimental protocol shows remarkable improvement in mass data transfer to a large number of farm machines.

Technology Refresh of the BNL Data Network. *TEJAS JAGANI (Rutgers University, New Brunswick, NJ 08901) AJ TEMPROSA (Brookhaven National Laboratory, Upton, NY 11973).*

The Network Operation Group (NOG) in the Information Technology Division at Brookhaven National Laboratory (BNL) designs, implements, maintains and performs technology refresh on the campus network infrastructure. This paper will briefly discuss the network infrastructure upgrade at BNL from hubs to managed switches, in this particular case Building 326 (Site maintenance) and Building 423 (Vehicle maintenance). It will describe the migration from shared media to switched media. Included in this upgrade is an upgrade from Asymmetric Digital Subscriber Line (ADSL) to a Fast Ethernet uplink. It will also give the NOG increased remote management monitoring capabilities. This will provide a 1000% increase in available bandwidth and increased available port count for the end users and terminal devices.

Detecting Patterns in Pseudo-Random Numbers. *ANDREW JENNINGS (Arizona State University, Tempe, AZ 85287) LIZ FAULTERSACK (Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID 83415).*

There are many situations where it is useful for computers to act unpredictably. Unfortunately, it is impossible for them to do so because it is impossible for a computer to generate truly random numbers. Instead, pseudo-random number generators (PRNGs) use mathematical formulas to generate sequences of numbers that are random enough for most purposes. Many security systems have been compromised by the subtle patterns still inherent in these pseudo-random sequences. Our research collected information about IP port scanners as they probed the INEEL network and sought to associate their scans with patterns of common pseudo-random number generators. Some IP port scanners use pseudo-random methods to choose their targets, presumably to obfuscate their activities and escape detection. Two common PRNGs, linear congruential and LFSR-based, are described along with methods to identify patterns indicative of those generators. More algorithms are developed which account for common complications in collecting the sequence as it was produced by the PRNG. These include algorithms for an observer who only has access to every n th number in the sequence and algorithms for an observer who receives a sequence that has been scaled (integer division performed and the remainder lost). So far, no identifiable PRNG patterns have been discovered in the INEEL port scan data, but ideas for enhancing these algorithms to be more network-tolerant are proposed.

Improving GIS Data Management for LandScan Global Population Projects. *KEVIN JOHNSON (University of Tennessee, Knoxville, TN 37996) BUDHENDRA BHADURI (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

The gathering and organizing of spatial data is essential for having quick access to appropriate information. The LandScan Global Population project is supported by National Imagery and Mapping Agency (NIMA) records on 11,000 CD-ROMs that contain scanned maps and aerial images throughout the world. To determine what areas are covered by this information, a worldwide map index was created in a Geographic Information System (GIS) based on coordinate positions. This process provides an efficient visual representation and enables a simple automated search via the map to retrieve the appropriate source information. LandScan USA is a project that looks at daytime and nighttime population distributions. Data for schools, prisons, and tourists are critical in developing daytime population distribution. Schools and prisons are commonly found in every county,

and two general databases that included these data for the entire United States were located. Unfortunately, no GIS metadata were available for either database. Also, about 30.5% of schools in the database lacked coordinate positions. Using Census block data, TIGER roads, and a street atlas an attempt was made to locate the prisons in a 29-county study area around Houston, Texas. This method had an approximate 50% success rate. Some prisons lacked a street address, and some locations were not supported by the population reported in the Census data. Other data collection techniques were explored for the Washington, D.C. area to gather information regarding people visiting and working at museums and businesses.

Configuring Microsoft Windows XP Operating System for End User Operation in the Environmental Molecular Science Laboratory. *RICHARD JOHNSON (Columbia Basin College, Pasco, WA 99301) SCOTT CAMPBELL (Pacific Northwest National Laboratory, Richland, WA 99352).*

Computers are widely used in laboratory environments for purposes of data retrieval, data analysis, communication, and implementation. A secure, stable environment is necessary for users to utilize computers in a productive environment. Pacific Northwest National Laboratory (PNNL) requires reliable computers for researchers to be most effective. To facilitate installation of Microsoft Windows XP ("Microsoft Knowledge Base Article " Q314459", 2001) and place it on the domain, an unattended installation answer file was preconfigured insuring a uniform and secure installation ("Microsoft Knowledge Base Article - Q308662", 2001). Using the above methods resulted in a consistent, stable, and secure environment that is optimal in supporting needs of scientists in a supported laboratory. Not only did this method result in a stable and secure environment it provided a rapid roll out time for computers placed on the domain. Success using unattended installation disks along with Microsoft Windows CDs leaves interesting research opportunities in using network installations, not only to speed up deployment, but also to allow installation of Windows XP anywhere on the PNNL's domain.

Online Ceramic Waste Form Database. *JULIE KIENTZ (The University of Toledo, Toledo, OH 43606) THOMAS FANNING (Argonne National Laboratory, Argonne, IL 60439).*

In order to determine if the Ceramic Waste Form is acceptable for the proposed Yucca Mountain repository in Nevada, radionuclide release modeling is being performed. Two types of tests involved, pH Buffered tests and Solution Exchange tests, produce large amounts of experimental data that is currently being recorded into various scientific notebooks and computer files. Individual experimenters perform calculations on the data and record the data similarly. By creating a database for these two types of tests, all of this information will be in a single, consistent storage space that is easily accessible for all individuals interested in viewing the data. In addition to a centralized data location, the database can be used to perform all of the complex calculations involved to ensure they are all calculated the same way and reduce the possibility of human error. The database has been created using Oracle and the Structured Query Language. To make the database more useful, a web interface has been created using the programming language Perl's Database Interface and Common Gateway Interface capabilities. This web interface will contain menus and links that will allow experimenters to easily search the data, navigate through different sets, and compare information with similar attributes. Although there is still more data to load, the database, web interface code, and documentation have been completed.

Porting of RTEMS (Real-Time Executive for Multiprocessor Systems). *JENNY KIM (Suffolk County Community College, Selden, NY 11784) D. PETER SIDONS (Brookhaven National Laboratory, Upton, NY 11973).*

RTEMS is an open-source real-time executive, which is ideally suited to embedded microprocessor applications (i.e., applications in which a computer is buried inside a device). Examples of such embedded systems are cellular phones, PDA's, and common household appliances such as a kitchen stoves and microwaves, and also VCR's and TV's. These devices are also used by scientists for collecting and analyzing physical data from transducers, and for controlling the instruments that make the measurements. General operating systems such as Windows are not suited to this task, since there are often time-critical operations, which must happen on-schedule or even on-

demand with a short-time latency. This is the purpose of a real-time operating system (RTOS), and RTEMS is such a system. Although this system has already been ported to several CPU families, including the Motorola 6800 series (of which the MCF5272 is one), each member of the family and each hardware configuration involve detailed changes that must be addressed for the system to work. This system-specific code is referred to as a Board Support Package (BSP). This project aims to generate a BSP for a commercially available microprocessor board, the uCDimm. This finished product will be an embedded control system for a sophisticated x-ray detector to be used at the National Synchrotron Light Source.

Automated Analysis of Tryptic Peptide Tandem Mass Spectrometry Data with a Perl Programming Language Script.

ANGELO KONTGAS (*Salt Lake Community College, Salt Lake City, UT 84130*) WILLIAM CANNON (*Pacific Northwest National Laboratory, Richland, WA 99352*).

A large body of tryptic peptide data has been generated through the use of electrospray ionization (ESI) collision induced dissociation (CID) tandem mass spectrometry. (MS/MS). More than 1 Terabyte (TB) of such data is stored in data servers at Pacific Northwest National Laboratory (PNNL). Manually extracting specific tryptic peptide spectra from that data can be particularly tedious, as the focus data are generally spread across many different collections. The "Proof of Concept" solution incorporates a method to achieve a virtual file transfer of data from the remote server and conduct a mandatory linear search of these large text files. To eliminate the manual search requires investigation of methods to automate the data transfer, fragment analysis, and a graphical presentation of the results. A fully automated search of the peptide database repository for 10 spectra with seventeen amino acids was accomplished. Those isolated spectra data served as input for a MatLab based analysis program that generates a graphical representation of the postulated fragment analysis of the peptide. This work will, in part, enable large-scale data mining of MS/MS data in order to develop advanced computational analyses. These advanced analyses will lead to statistically rigorous algorithms for identifying peptides and proteins obtained from complex cellular extracts.

A Graphical User Interface for a Scanning X-ray Microscope.

NATHAN KRAPP (*University of Chicago, Chicago, IL 60637*) PATRIC DEN HARTOG (*Argonne National Laboratory, Argonne, IL 60439*).

The Scanning X-ray Microscope (SXM) located at the 2-ID-B insertion device at the Advanced Photon Source (APS) is used by both Argonne employees and outside users to use the brilliant x-rays provided by the APS to determine details about the structure of objects on a scale smaller than what is achievable at many other facilities. Because the APS can produce x-rays of higher brilliance than any other facility currently in existence, this is a valuable tool that should be used as efficiently as possible. However, the current interface for dealing with this microscope is very inefficient, as it is complicated for users to learn, and can cause up to 12 hours in a 24 hour period to be lost when setting up a scan, a waste of valuable beamtime and resources. The purpose of this project is to provide a clear and concise graphical user interface (GUI) written in the IDL programming language that will bring all of the different components necessary to make a scan together into one window, where a user can quickly and efficiently take and view scans without having to learn anything about the more complicated underlying structure. The goal is to go from wasting 50% of the beamtime setting up scans to as little as 10%, and also to provide many features that are currently unavailable, such as saving additional information, and viewing scans as they are made, in real time.

Testing the KOPIO Detector Design by Visualizing a Simulated Run with OpenDX. RACHAEL LESHNER (*Jamestown Community College, Jamestown, NY 14701*) GORDON J. SMITH (*Brookhaven National Laboratory, Upton, NY 11973*).

Whenever large amounts of money are to be spent on building a vital piece of research equipment, it is always best to make sure that the device will function as needed before it is built. In the case of the KOPIO detector design, visualizations of simulated runs were determined to be the most feasible method to accomplish this goal. OpenDX, being open source and highly customizable, was determined to be the most cost effective and efficient program for the task. Visualizations of the data were created in two forms. One displayed a particular azimuth and elevation for all the z-coordinates, while the

second displayed all the azimuths and elevations for just one z-coordinate. Both were equipped with sequencers so that the program could automatically progress through all the angles or z-coordinates, respectively. Areas of low detection were easily recognizable, and thus the goal of the project was accomplished.

Standing Wave Linear Accelerators: An Investigation of the Fundamental Field Stability and Tuning Characteristics.

ELLIE LIN (*University of Texas at Austin, Austin, TX 78712*) ROGER M. JONES (*Stanford Linear Accelerator Center, Stanford, CA 94025*). Field stability and tuning are critically important for the design of any accelerator. The standing wave structure is under consideration for implementation in the Next Linear Collider. A 15-cavity standing wave accelerator structure was modeled with equivalent circuits in which nearest neighbor coupling was incorporated in the model. Operation in the p and p/2 modes of acceleration was analyzed. To simulate fabrication errors, random and systematic frequency errors were added to the cavities and then subsequently minimized by tuning the first, middle, and last cavities. The p mode of acceleration was found to be more sensitive to errors than the p/2 mode of acceleration. Tuning only three out of an available fifteen cavities was successful in minimizing the errors in the field flatness. The dipole wakefield was also studied for the standing wave structures and compared to that in traveling wave structures.

Producing a GUI (Graphical User Interface), and Making a Single User Program Multi-user. ANDREW LOBBAN (*Richard J. Daley College, Chicago, IL 60652*) MIRIAM BRETSCHER (*Argonne National Laboratory, Argonne, IL 60439*).

The Pager program was written by Iain Tilbrook to serve him personally, and I had been assigned the task of modifying this same program to accommodate the Argonne Community. Specifically, I was given the job of produce a GUI using a web development language called PHP. The programs files (scripts) are to be written then stored on a Unix server called Sarasate. Another program exists on the same server (Maple) as the database, which reads the Oracle database, but there isn't an interface to write to that database; consequently, the declared project was to create the interface and transfer them to the server folder on Sarasate. Equipped with a PC and little developmental tools installed, some basic designs were acquired. But in order to produce these scripts faster and better, another developing tool "Dream Weaver MX" was taken into consideration. Having no prior knowledge about Web Development, tutorials (Books and Internet Resources) were used for reference, and co-workers were interviewed for additional information. When a script is developed, it has tested before it is transferred to the Sarasate. The program was created using the logical procedure of any program: A Login Screen, Data Input and Data Process Screens. With steps in mind, a web-based design was drafted. Each design has to be easy to manipulate to accommodate non-computer and computer users; that is why the designs had to be made simple and straightforward as possible.

Spectral Element Multigrid Methods. JAMES LOTTES (*University of Illinois at Urbana-Champaign, Urbana, IL 61801*) PAUL F. FISCHER (*Argonne National Laboratory, Argonne, IL 60439*).

A new scheme is developed that solves many of the problems faced by spectral element multigrid methods. This scheme, the LCS algorithm, is a multiplicative domain decomposition approach tuned for application to spectral elements. Like pure spectral methods, spectral element methods are high order, yet they enjoy the same flexibility for handling complex geometries as finite element methods using linear basis functions. Much work has been done to develop fast iterative linear solvers for the systems of equations resulting from spectral element discretization. Some of this work has been to extend the multigrid class of algorithms to spectral element methods. In 2D and 3D, the Gauss-Lobatto node spacing of the spectral elements creates high aspect ratio cells, a well-known source of difficulty for multigrid algorithms. A range of spectral element methods incorporating multigrid ideas are analyzed and compared to the new method. The LCS method is shown to reduce the work required by the fast previously used method by a factor of 2.5.

Systems Management Projects: Contacts List, SSH, and Proxying Web Caches. CORY LUENINGHOENER (*University of Nebraska Lincoln, Lincoln, NE 68508*) REMY EVARD (*Argonne National Laboratory, Argonne, IL 60439*).

Systems administration is a research area that is often neglected in the overall realm of Computer Science. There are, however, a large number of problems that arise while keeping computers running smoothly. Effective management of SSH (Secure Shell) keys is one such problem. SSH keys are meant to be permanent pieces of data for a host and need to be saved/restored when a computer is rebuilt. This requires a database to hold the keys and some scripts to keep the database up-to-date. Efficient transferring of data between computers on a network through use of a staging model is another open problem. One idea is to use a proxying web server to cut down on load. Managing to work on these problems while helping keep all of the computers in a workplace running and not going insane is a real problem in the world. These problems and more are discussed in a friendly, easy-to-read format.

Scalable Systems Software Project. *ANDREW LUSK (University of Illinois at Urbana-Champaign, Urbana, IL 61801) NARAYAN DESAI (Argonne National Laboratory, Argonne, IL 60439).*

In the field of high performance computing, the most popular new area is that of the "commodity supercomputer": a cluster of hundreds or even thousands of computers made from off-the-shelf components. The low cost and high performance of these clusters has resulted in their sizes growing recently to thousands of nodes. The downside is, with the sheer number of computers involved, these clusters can become management nightmares. Argonne is one of the laboratories that are participating in the Scalable Systems Software project, which aims to provide a comprehensive set of tools and libraries to make cluster management and the development of new tools for cluster management much easier and more standards-based than it currently is. The modern cluster needs several components to do daily use and/or administration tasks, as well as provide fault tolerance. The components themselves need message framing abstractions to give the user of the Scalable Systems Software distribution choices when implementing authentication and outside components that hook into the system. Argonne's contribution has been a component for running programs on a cluster, a component that manages administration tasks for a cluster, a component that handles asynchronous events and fault tolerance, the central service directory that allows components to locate each other, and the underlying communication library that abstracts away arbitrary wire protocols from the components. This allows drop-in changes of communication protocols transparently to the system. The culmination of this research is deployment of the Scalable Systems Software tool kit on Argonne's scalable cluster test bed, Chiba City.

Protocol Design and Implementation for Highly Mobile Robot Networks. *ARUL MANICKAM (Carnegie Mellon University, Pittsburgh, PA 15213) NAGESWARA S. RAO (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

Traditional network infrastructure is not well suited for mobile wireless applications where connection quality varies frequently and links between nodes are constantly being made and broken. This project implements a novel protocol, called Connectivity-Through-Time, that enables communication in a dynamic wireless network by using the nodes to route and buffer messages. A group of robots running Linux OS equipped with 802.11b ethernet cards were used in the development and testing of the protocol. The first advance over traditional networks is the use of buffering when the destination is unreachable via physical links, be it single or multiple hops. Data can then be delivered at some later time if some nodes previously connected either via physical links or through time to the sender come into contact with the destination. Another improvement over traditional networks is the use of UDP rather than TCP. TCP can only be used to transfer data between two nodes. For wireless networks, however, when the destination is unavailable it is desirable to transfer the data from the sender to all nodes within range as efficiently as possible. UDP provides a mechanism for this in that it allows messages to be broadcast to everyone on a local network at once. In addition, flow control can be managed at the application level. This is necessary since TCP does not distinguish between traffic congestion and physical layer losses due to radio problems. This protocol shows promise of an efficient robot network in highly dynamic and unpredictable environments.

CyberSecurity: Windows Remediation. *AMIN MATEO (Suffolk County Community College, Brentwood, NY 11717) MICHAEL STANGEL (Brookhaven National Laboratory, Upton, NY 11973).*

The essence of a laboratory is its developments, and in order to keep these important information from falling into the wrong hands you'll need security, especially now a days with the new technology such as the internet. Not keeping up to date with the right software can be vital to the safety of the scientist's sensitive data. The departments System Administrator (SysAdmin) monitors each computer that is connecting to Brookhaven National Laboratory (BNL) network. Once there is a problem that the SysAdmin can't handle or us at Information Technology Division (ITD) needs to examine their Computer, on one occasion remediation of their machine. When an ITD specialist is in front of the computer, they have tools and many steps to take to ensure that the remediation is done properly. If we do one computer we make sure that the whole department gets done. We also setup new computers for BNL's workers, and made sure they are connecting to the BNL's Network. In order, for them to be connected we had to make custom-made CAT-5 cables for the computers, which need to organize in color sequence. Setup and installed Windows 2000 on over 250 computers.

Investigation of MPI Performance in Parallel Linear Algebra Software on Linux Beowulf Supercomputers. *VYTAUTAS MIRINAVICIUS (State University of New York at Stony Brook, Stony Brook, NY 11794) JAMES DAVENPORT (Brookhaven National Laboratory, Upton, NY 11973).*

As the need to solve high scale computational problems increases, more computing power is required. For this reason a supercomputer has to be used. What defines a supercomputer is a collection of processors that are able to communicate with one another. To utilize a supercomputer MPI (Message Passing Interface) has to be implemented. The challenge in designing efficient algorithms using MPI lies in a programmers' ability to divide the problem into reasonable chunks so that these chunks could be sent to each processor in the most efficient way. In this research project the performance of several MPI (Message Passing Interface) functions on three Linux Beowulf clusters was measured. First a single processor of each cluster node was tested by running a matrix multiplication program. Then a parallel implementation of the matrix multiplication program was executed. In the next stage of the project SkaMPI (The Special Karlsruhe MPI-Benchmark) was deployed. In the final stage PETSc (The Portable, Extensible Toolkit for Scientific Computation) software was installed and used to solve a linear system of equations in parallel. The MPI send function slowdown was recorded for short messages in the matrix multiplication example and SkaMPI on the gigabit network compared to the ethernet network. However when the MPI messages sizes reached 1000 bytes there was a significant increase in MPI performance on the gigabit network. MPI performance in PETSc software did not indicate any significant improvement on the two networks. Future research modifications were suggested to improve the performance of these MPI functions.

Rewriting of the Integrated Operations System Using New Technology and Techniques. *ADAM MITCHELL (Washington State University, Pullman, WA 99163) TODD ELSETHAGEN (Pacific Northwest National Laboratory, Richland, WA 99352).*

Pacific Northwest National Laboratory uses the Integrated Operations System, a web-based application, supporting their Environmental Safety and Health (ESH) program. IOPS helps promote a safe and productive working environment for staff at the laboratory. IOPS controls laboratory access, communicates hazard information, and assigns and tracks training based on a staff member's interaction with hazards. The Integrated Operations System, or IOPS, was first written in 1997. Since then, IOPS has expanded greatly. As the total amount of code grew and changed, the code began to include inefficient and unnecessary code. Additionally, file dependencies became so overbearing and circular that, often, nearly every file of the application was loaded to perform even the simplest of tasks. All of these problems caused the application to perform very slowly. To increase the speed of the IOPS application, it is being rewritten, almost from scratch. In the new environment, the main goal is to improve efficiency while maintaining usability. To achieve this, many new technologies and techniques are being employed. When the rewrite is complete, the application will look nearly the same to users, but will include substantial improvements. Some of these include: greatly increased speed and shorter load times; greater ease of maintainability; cleaner, more consistent look; as well as minor GUI improvements.

Creation of a Computerized Interface to Control a Deposition System Subset using LabVIEW and FieldPoint. EDUARDO MOUTINHO (Colorado School of Mines, Golden, CO 80401) RAMESH DHERE (National Renewable Energy Laboratory, Golden, CO 89401).

LabVIEW is a powerful programming tool that is used primarily with control equipment. The revolutionary aspect of LabVIEW is that it is a completely graphical programming language, which makes it easier to use than its text-based counterparts. This ease-of-use allows for much quicker program development. More importantly, this facilitates the development of software for complex systems. For example, LabVIEW can be used to create a program to control and automate a thin-film deposition system. In this case, a virtual switchboard can replace the mechanical one on the system. This is advantageous in many ways. For example, space needed for hardware can be reduced. And sequences can be programmed, which eliminate the need for scientists to stay and operate equipment for extended periods of time. Different sequences can be activated by a simple series of mouse-clicks. Also, automation minimizes problems caused by human error. In this project, we demonstrate how LabVIEW can be used for process control by simulating a subset of the actual process that a 3M deposition system goes through. This subset consists of external circuitry designed to simulate actual process operations, including that of valves, manometers, and interlock switches. LabVIEW will communicate with this circuitry using FieldPoint.

Using WIRED to Study Simulated Linear Collider Events.

AYODELE ONIBOKUN (Bethune Cookman College, Daytona Beach, FL 32114-3099) TONY JOHNSON (Stanford Linear Accelerator Center, Stanford, CA 94025).

The purpose of this project is to enhance the properties of the LCD WIRED Event Display. By extending the functionality of the display, physicists will be able to view events with more detail and interpret data faster. Poor characteristics associated with WIRED can severely affect the way we understand events, but by bringing attention to specific attributes we open doors to new ideas. Events displayed inside of the LCD have many different properties; this is why scientists need to be able to distinguish data using a plethora of symbols and other graphics. This paper will explain how we can view events differently using clustering and displaying results with track finding. Different source codes extracted from HEP libraries will be analyzed and tested to see which codes display the information needed. It is clear that, through these changes certain aspects of WIRED will be recognized more often allowing good event display which lead to better physics results.

Visualization with the DICOM File Format. SARAH OSENTOSKI (University of Nebraska Lincoln, Lincoln, NE 68588) MIKE PAPKA (Argonne National Laboratory, Argonne, IL 60439).

In the medical field, machines that take in data as digital images have become increasingly popular due to diagnosis many illnesses. This increase in the use of computers and digital imaging has led to a need for programs that can utilize the data coming from medical devices. Our project looks at the DICOM standard and methods of using this information in common visualization toolkits.

A Windows Based Interface for ALICE-91 (Fortran): Statistical Model Code System with Fission Competition. UNNATI PATEL (Rutgers -The State University of NJ, Newark, NJ 07102) DAVID SCHLYER (Brookhaven National Laboratory, Upton, NY 11973).

The assignment is to develop Windows based interface for ALICE91 developed to predict nuclear reaction cross-sections. The interface between ALICE91 input file and a Windows based environment would provide the user-friendly environment to input required data for the calculation. The program will be used to calculate radioisotope yields for reactions of medical interest, particularly in the future proposal of Proton Radiation Therapy Facility at BNL. Proton therapy is a precise form of radiation treatment. The main advantage is it primarily radiates the tumor site while minimizing dose to surrounding tissues and organs. Conventional radiation often radiates healthy tissues reaching and surrounding the tumor site. Chemotherapy goes throughout in the body, unlike radiation and surgery, which are considered "site specific" treatments. The program ALICE91 along with FLUKA, SRNA-2KG, etc will be used to gather data on known cross-section and stopping powers. The program input file is written in C++ allowing it to be displayed on MS-DOS and creates an output file with user opted

variables. The C++ created output file will be used by ALICE 91 source code written in FORTRAN to perform the calculations.

The ATLAS Experiment. JASON PERRY (Monroe Community College, Rochester, NY 14623) KÉTÉVI A. ASSAMAGAN (Brookhaven National Laboratory, Upton, NY 11973).

The ATLAS Experiment is a global initiative to develop a large sub-atomic particle detector. It is a massive effort demanding the expertise of approximately 2000 physicists worldwide. Brookhaven National Laboratory physicists, among other things, have been working on a special part of the ATLAS Detector called the Cathode Strip Chambers (CSC). The main task for this internship was to develop computer programs using several software applications that would give scientists and researchers web-access to a database application, which would house testing results for the CSC. An object-oriented language, LabVIEW, was used to create a program that would switch the existing data from previous tests from .dat extension to a new Access database table format. LabVIEW was also used to change existing testing programs into a format that would write the results in an Access database table automatically, no longer writing them in a .dat extension format, and automatically saving the front panel of the test that was run for future reference. Next, a Visual Basic application was developed to arrange the test results in a user-friendly format and provide some helpful features such as statistical tools and images for scientists and researchers to be able to analyze test results from the database. A web page was then constructed using Dream Weaver 3 software that contained a summary of the database application and a link to enable scientists and researchers to download it.

Extending and Implementing EPICS IOC Core for Diagnostics Systems. NICHOLAUS PONGRATZ (University of Wisconsin, Madison, WI 53706) SAEED ASSADI (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The work of this project primarily deals with the benefits and issues of installing and using EPICS IOC Core with laser-wire beamline measurement systems, though the work is applicable to all diagnostics. Like most organizations, the SNS Diagnostics Group is in the classic position of increasing performance of their systems while keeping costs, maintenance and deployment time low. It was determined that leveraging the commodity hardware and software market was the best choice for implementing their systems, rather than using high-cost custom solutions. EPICS on Microsoft Windows was chosen as the software platform because EPICS is a standard control system used throughout the industry, and Windows provides acceptable performance with few advanced customizations required. New high-end oscilloscopes, such as the Tektronix TDS7404, come with Windows built-in. As such, these scopes running IOC Core provide a very convenient platform for data acquisition, analysis, and publication. Rackmounted computers running Windows XP Embedded on x86 hardware complete the commodity-based system by connecting to the EPICS databases and providing further analysis. A prototype system integrating these elements was constructed. Though building IOC Core for these systems is a fairly straightforward process, important modifications for successful implementation are discussed. The role of Shared Memory, a new mechanism for serving data to the world via Channel Access, is also discussed. While this work has been primarily focused on laser-wire systems, the success of this implementation suggests that it will be considered for many future projects within the SNS Diagnostics Group.

Grid Computing. HECTOR RODRIGUEZ (Pace University, New York, NY 10013) GREGOR VON LESZEWSKI (Argonne National Laboratory, Argonne, IL 60439).

My contribution to the project consist of helping in the development of what is called the Java CoG Kit, the Java CoG Manual and the development of a website using PHP. The purpose of my internship was to focus more on education then the development of any projects. I entered this program with little knowledge of programming and Grid Computing. Grid Computing is an infrastructure that provides a linkage of resources so that scientists may collaborate their work. My fellow team members and I worked on a way to ease the installation of the Java CoG Kit for the Grid community. The purpose of this component is to allow users of the CoG kit to install and setup all necessary components via a user-friendly graphical application. I

have been given the opportunity to learn interesting and useful technologies hands on. Such tools include ANT, JDK 1.4 and CVS. Now I am able to collaboratively develop code within a work group. I intend to perform and utilize these new-gained skills as part of future computer science activities within my degree program and personal company.

Single Axioms for Ortholattice Theory and Orthomodular Lattice Theory. MICHAEL ROSE (Ohio State University, Columbus, OH 43210) WILLIAM W. MCCUNE (Argonne National Laboratory, Argonne, IL 60439).

Short single axioms for ortholattice theory and orthomodular lattice theory are given in terms of the binary operation, Sheffer stroke ($_ _$). Also $((y \mid x) \mid (x \mid z)) \mid u) \mid (x \mid ((x \mid ((y \mid y) \mid y)) \mid z)) = x$ is proven to be the shortest single axiom for ortholattice theory in terms of the Sheffer stroke with length 23 and 4 variables. Two theorems in the literature restrict the structure of possible single axiom equations allowing for the systematic generation of candidate equations. For the ortholattice single axiom, candidates were filtered through an ortholattice identity decision procedure and tested on a set of non-ortholattice models. With the resulting equations, proofs were attempted using Otter (W. McCune, 1994), an automated deduction system for first-order logic with equality. Promising candidates were focused upon, and complete proofs were found by Otter. The orthomodular lattice axiom was found similarly.

Dynamic-C Programming with a RCM2100 Board. JOVAN SPARACINO (Richard J. Daley College, Chicago, IL 60652) ISTVAN NADAY (Argonne National Laboratory, Argonne, IL 60439).

Embedded control systems are used in industrial systems, consumer products, and electrical appliances. They are programmed to do a task and than have the task burned into the ROM/Flash and embedded into the system. The Rabbitcore RCM2100 is a programmable microcontroller designed with its own computer language, Dynamic-C. Dynamic-C contains all of the C language functions and over 200 of its own functions designed for the Rabbitcore modules. Some of the features of the RCM2100 are its Ethernet ports and is able to act as a web server. A developing trend in technology today is creating measuring instruments that are used over the web. These have many advantages over the normal instruments. One of the most important is the easy of collecting and storing of data from them. The goal of this project was to design a program that would allow an electrometer to send its readings from a remote circuit board to the RCM2100. The RCM2100 would act as a web server to transmit to any computer on the Internet that can then display the readings on a webpage. Despite gaining much knowledge and experience from the research there still is some work that needs to be done.

Electronic Document Management System. KERBY ST.CHARLES (Miami Dade Community College, Miami, Florida 33167) VYTENIS MILUNAS (Argonne National Laboratory, Argonne, IL 60439).

Plant Facilities Services Division (PFS) at Argonne National Laboratory, is responsible for maintaining the laboratory's building infrastructure (e.g. buildings, roads, grounds, site utilities, and disposal facilities). How can a division be responsible for managing and maintaining internal general purpose of building systems such as structural, mechanical, and electrical on a limited budget maintain itself? PFS faces a challenge. It is inefficient and ineffective to handle our paper documents. First of all, paper document can be out of date even before distributed. Second, revisions of paper documents are costly, particularly for those requiring frequent updates. Third, facility costs for keeping paper archives are substantial. Last, but not the least, paper documents or drawings are susceptible to aging and damage over time. Although we have seen those challenges in handling paper documents, adoption of an electronic process may prove a challenge, if not the largest one especially in the engineering process. The concept electronic document management system is a multimedia conceptual design tool. Its goal is to provide design teams with easy access to information. With that goal in mind a team of information professionals started a project to restore the stick set room, which is a room we store all the drawings. Several hurdles were overcome, and several remain. This paper discusses the history of the project and its current status.

Interpreted Languages for Parallel Systems. MICHAEL STEDER (Elgin Community College, Elgin, IL 60123) ROBERT JACOB (Argonne National Laboratory, Argonne, IL 60439).

The goal of the National Science Foundation research project jFlexible Environments for Grand Challenge Climate Simulations is to help develop tools that will make it easier (flexible) to solve the most difficult problems of climate science. FEGCCS is looking into integrating an interpreted language into their climate model's to aid in development and control/visualization of the climate system. Before an interpreted language can be used in such an important capacity its performance has to be verified through testing of communication routines using different programming languages and networking protocols. Python was chosen as a likely candidate due to its previous use in science applications. Tests were designed and built from code already being used at Argonne and the tests were run on the laboratories 300+ node Linux cluster known as Chiba City. After analysis of the data it was clear that Python would perform in a parallel system. Python shows great promise for helping to modernize and accelerate climate research on computer clusters.

Creating a Dynamic Web-Administrated News and Event Management System Using Open Source Technologies for the Environmental Sciences Division of Oak Ridge National Laboratory. AARON STEWART (Rensselaer Polytechnic Institute, Troy, NY 12180) LINDA ARMSTRONG (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The Environmental Sciences Division (ESD) of Oak Ridge National Laboratory (ORNL) communicated heavily with E-mail bulletins and web news pages. The former were sometimes lacking in depth, and updating the latter's HTML was time consuming. The ideal solution appeared to be an inexpensive system that could be administrated easily, and accessed remotely. An Apache web server, with the powerful PHP scripting language enabled, and an accompanying MySQL database were installed, configured, customized, and hardened on existing ESD hardware. Using the PHP scripting language, a series of web pages were programmed that not only updated themselves based on database information, but provided a layer of abstraction to the database, enabling staff to edit, update, remove, search, and administrate news announcements, upcoming seminars, and perform specialized printing without ever having to leave a simple web form interface. Actual adoption of the service(s) by staff was mixed and improving at the time of writing, but the project represents a certain great technical success; hardware that was essentially taking up space became a provider of useful services running software that is efficient, scalable, and compatible with no additional costs to ESD. For some needs, web applications can epitomize good software: portable, accessible, relatively easy to design, and making a particular task easier and faster to do. Open source products such as Apache, PHP, and MySQL are powerful tools for such projects and should not be considered lightly by institutions or businesses in need of such services.

Web Development in the Lotus Notes/Domino Environment. ROHIT TANDON (Gonzaga University, Spokane, WA 99258) MARY SUE HOXIE (Pacific Northwest National Laboratory, Richland, WA 99352).

Although offering similarities, Lotus applications do not work the same as relational databases. Web development in the Lotus Notes/Domino environment allows for the creation of dynamic web pages, which use fields to store data into documents. These documents then can be queried in a variety of ways to present relevant data to end-users. During my time at PNNL I was able to learn Lotus Notes/Domino and create additions to and edit several existing web sites. These sites are used by both the Office of Fellowships and the Department of Energy Science Education Program and contain data used in the hiring of fellows and interns.

Network Architecture: Wiring Topologies, Transmission Media and Security of the Network. HEATHER THOMBS (BMCC, New York, NY 10010) KEN TERRY (Brookhaven National Laboratory, Upton, NY 11973).

Even before the Internet was popular the idea of communicating was always at use with humans. When it came to sending messages there was system with how it would be brought form one person to another. Some of ways that we communicated consisted of some signals, notes tied to birds, Morse code and horse back rides who delivered

information from one town to another. It has long come to an idea of how communication can be effective in an environment that works with various types of information. In recent years the communication field has since grown to a better architecture of technology. There have since been various communication devices that we use in our everyday lives such as the telephone or a computer. By the use of these devices, information is much easier to obtain. The network architecture can bring the information not only easier but also faster and secure to where it would be needed or used. In networking the term Topology refers to the layout of connected devices on a network. In a LAN (Local Area Network) there are 3 common types of typologies used to map out how information will travel through the network, they are the following: Bus, Ring and Star. Each typology is some form of logical or physical arrangement that is used in the media structure for a building or a school campus. By using a blueprint or map of a building or a campus, a topology can be arranged to begin the wiring methods used to build the network for better communication.

Using ION to Create Graphs from NetCDF Files for the ARM Project. BRADLEY THONNEY (*Walla Walla Community College, Walla Walla, WA 99362*) MATTHEW MACDUFF (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Network Common Data Format, or NetCDF, files, while extremely efficient, are very difficult to read and understand. When scientific data is entered into NetCDF files, interpreting software must process these files. The software outputs data in a graphical format that is easy for the scientists to understand. Due to the need for real time data, it is vital that computers process information as efficiently as possible. In order to ensure efficiency it is necessary to explore all the options available. The most recent option to become available for writing these programs is ION (IDL On the Net). The goal of this project is to write a program, using ION that is comparable to programs already in place such as ANDX (ARM Network Data Extract). This program is able to graph data from multiple dates and displays clear and easy to read graphs.

Linux Configuration Performance Evaluation for HPC Linux Cluster. TOBY TRUJILLO (*New Mexico Highlands University, Las Vegas, NM 87701*) REI LEE (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The performance of individual compute nodes in a High Performance Computing (HPC) cluster is vital to overall system performance. In the development of a HPC cluster there are many different variables to consider in order to have an optimized configuration. The obvious considerations for the nodes of a supercomputer cluster are that of hardware and software. Along with these considerations it is also important to have data on how each of the hardware and software components work in different environments. To accurately test the performance of different system configurations a variety of benchmarks were used to gather data for the evaluation process. Each of these tests was performed using many different combinations of hardware and software environments and yielded the ideal system configuration for high performance parallel computing. With the knowledge of the performance of different configurations, constructing a high performance cluster can be managed much more easily.

Finding Optimal Conditions Using A Genetic Algorithm In FLOW. DIANE VIAN (*Ball State University, Muncie, IN 47306*) JUAN J. FERRADA (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Simulating a chemical process offers an opportunity to view the outcomes of the process before doing the actual experiments. Analysis of the results provides insight into the cost and performance of the process. This analysis can be used to determine the best conditions under which a process will work. Simulating a process allows for a good analysis of the safety, ecological and economical outcomes. FLOW is a DOS-based program that simulates such processes and was created and is currently used at Oak Ridge National Laboratory. FLOW is capable of simulating processes and analysis can be made based on sensitivity or uncertainty parameters. The addition of a feature that has the capability to optimize a process, hence increasing the usefulness of FLOW, is the desired outcome of this project. This feature uses the mathematical tool of a genetic algorithm to optimize a function and incorporated work done by David Coley in An Introduction to Genetic Algorithms for Scientists and Engineers. The genetic algorithm is being used to test a simple minimization problem, with a known solution, to understand the

properties and outputs of the genetic algorithm and the program. Determining a diameter that produces a minimum cost was selected as a simple problem to test the genetic algorithm. To accomplish this, the existing code was modified, put into FLOW and links were developed to use the two programs together. The ultimate goal would be to create a useable tool in FLOW that represents the process of finding the optimal results when there is more than one unknown variable.

Grid Services Flow Language. PATRICK WAGSTROM (*Illinois Institute of Technology, Chicago, IL 60616*) GREGOR VON LASZEWSKI (*Argonne National Laboratory, Argonne, IL 60439*).

The rapid development of the Internet over the past decade has spawned a large variety of non-interoperable services. With the development of Web services frameworks many of these interoperability problems have been solved. Learning from commodity tools, many components of computing Grids are beginning to utilize Grid-enabled Web services for interoperability. One major promise of the Web services architecture that has not been integrated into Grid services is compositability of multiple services into one aggregate service, a process known as workflow composition. In this paper we examine the background behind this problem, current solutions in the Web services world, and propose a solution that is suitable for Grid Services. This solution, the Grid Services Flow Language, is a robust XML based language that is based off Web service workflow languages and customized for Grid computing. We then discuss the preliminary implementation, based on evolving Web service and Grid service standards, and present ideas for future work.

Visual Models for a Data Architecture Study at Argonne National Laboratory. RITA WALTER (*Truman College, Chicago, IL 60640*) MIRIAM BRETSCHER (*Argonne National Laboratory, Argonne, IL 60439*).

Currently, Argonne Operations data exists in a mixture of complex hybrid IT environments, with internally developed or proprietary systems that are not as well integrated as they could be. As additional software solutions are introduced, the risks of interoperability conflicts increase. A common architecture is proposed that will standardize processes, components and tools, eliminate redundancy, and clarify business rules. The first step in this architecture study is to depict what currently exists, starting at a high level and deciding what methodologies are best suited to the purpose of uncovering data. A working Group was commissioned to define the top level or "core" data to clarify and selected two items to begin the investigation. The group then interviewed key players in the organization to uncover rules about this data. After the initial interviews, the data rules were assembled in a standardized format. Several different diagramming methodologies were chosen and employed to depict this core data: Activity (swimlane) diagrams, Repository diagrams, Venn diagrams, and a new type of diagram, a "data life" diagram were created. These particular methods were discovered as being most suitable for a clear depiction of core data at the highest level. Future work will employ the selected methodologies and expand the investigation to include other items of core data.

Improving the Accessibility of Physics Modeling Codes.

KATHERINE WHITE (*University of Tennessee Knoxville, Knoxville, TN 37916*) MARK CARTER (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Physics codes for modeling experiments are often difficult to use because of a lack of a graphical user interface (GUI), problems with performance optimization, and portability issues. All three of these problems were addressed in this project for the rant3d code, a FORTRAN code used to model antennas for heating plasma. The user interface of rant3d was previously text based and required the user to draw their antenna on paper before entering data into a text file. To improve this input method, a GUI was written in java. The GUI allows the user to draw different pieces of the antenna using the mouse, and the data from these drawings is then written to an input file for the FORTRAN code. Two methods were used to improve the performance of the rant3d code. Algebraic properties of Kronecker products were used to cut down on the number of operations performed. It was found Kronecker products could be implemented easily in some parts of the code, but it was not feasible to use these algebraic properties throughout the code. One piece of the code, which required a large amount of time, was computing two-dimensional fast Fourier transforms. To improve this section of the code, the Fourier transforms

were solved analytically, and the code was updated to use the analytical solution. To allow more users access to the rant3d code, the code was ported from IBM AIX to a Linux operating system. The result of this project was an optimized, portable rant3d code with a GUI front end.

Mapping the netCDF Application onto the Metadata Catalog Service. MARK ZAVISLAK (*Stanford University, Stanford, CA 94305*) VERONIKA NEFEDOVA (*Argonne National Laboratory, Argonne, IL 60439*).

The Metadata Catalog Service (MCS) is a project born out of a proposal to provide a highly extensible system that would make it easier for users to deal with large amounts of data dispersed through different files and collections. With the MCS, climatologists and climate simulation software, for instance, could have a central place with which data about a particular region could be found and queried among hundreds and thousands of data files spread across varying locations. The Network Common Data Format (netCDF) is one scientific data system that researchers hope to interface with the MCS. The 1.0 version draft of the Metadata Catalog Service was tested to see if it was compatible for efficient storage of the netCDF Markup Language (NcML). The specification, as it stood, was not sufficient to deal with this specific application. A variety of alternative methods were also discussed and tested, wherein it seemed that the best solution would have been to store the NcML in a manner that preserved its XML roots plainly as possible.

ENGINEERING

Preferential Oxidation Catalyst Testing in a Single Channel Catalytic Reactor. ADAM HEINTZELMAN (*Michigan State University, East Lansing, MI 48824*) KRISTON P. BROOKS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The efficiency of the polymer electrolyte membrane fuel cell (PEMFC) is highly dependent on the purity of the hydrogen fuel supply. Reforming hydrocarbons produces carbon monoxide (CO) in excess of the acceptable level for the PEMFC and essentially poisons the platinum anode catalyst. In order to achieve the Department of Energy (DOE) targeted carbon monoxide levels of 10 ppm, we have found preferential oxidation (PROX) to be an essential final step of the fuel processing. Through experimentation, two stages of PROX were found to be necessary: first stage PROX, which contains a non-precious metal catalyst run at an optimal temperature of 180°C, and second stage PROX, which contains a precious metal catalyst run at an optimal temperature of 100°C. Each stage of PROX was studied as functions of temperature, steam/gas ratio and O₂/CO ratios. Through these two processes it was observed that the DOE targeted CO levels of 10 ppm could be reached.

Ice Thickness Sensor Design. ISAIAH ABRAMSON (*Hebrew Theological College/ Illinois Institute of Technology, Chicago, IL 60659*) MARVIN KIRSHENBAUM (*Argonne National Laboratory, Argonne, IL 60439*).

One of the components in the Advanced Photon Source mechanical system is a water tank, which produces ice by tubes of liquid refrigerant running through the tank. The purpose of this project is to design, build, and test a new sensor that will monitor the ice thickness in the tank. The old sensor has many problems such as inaccuracy and it's difficulty to service. Due to these problems a series of new sensor designs are proposed that are durable, accurate, and easily installed and maintained. They consist of a sealed copper tube filled with water and a gap of air left for expansion. As the refrigerant tubes build ice, the water inside the sensor will freeze expanding into an air cavity, resulting in an increase of pressure. The pressure inside the copper tube is monitored by a pressure transducer and in turn measuring the amount of ice produced. In addition the only installation required is lowering the sensor by means of a rod into the tank. After a series of tests in a model ice tank, it was concluded that the above idea is effective in the given conditions of the tank and that sensor 3 is the most accurate in monitoring ice thickness.

Tele-autonomous Positioning of Robotic Manipulators. JAKOB ANDERSON (*Tulane University, New Orleans, LA 70118*) YOUNG S. PARK (*Argonne National Laboratory, Argonne, IL 60439*).

Precise positioning of manipulators is essential in performing many

robotic tasks. Much of a human operator's time is spent doing repetitive tasks that require a high level of accuracy. By automating these tasks, pressure is removed from the operator and a higher level of efficiency and precision is achieved. Automation requires the integration of sensors with manipulator control. By placing a laser grid over a target, a camera can capture geometrical positioning information. Using data about the current position of the camera and laser, it is possible to mathematically determine the coordinates of the target's normal vector. Kinematics routines are then used to determine the angles of the joints for the manipulator. The angles are then converted into commands that can control the individual motors of each joint in the manipulator. Many difficulties arose while trying to do the image processing and it is still unable to fully handle the required tasks. The kinematics work very well and provide a high level of accurate movement. The data acquired by the image processing can be directly used with the kinematics routines. A prototype is in development that will test these processes and help to refine them. Eventually it is hoped that this will be an addition to the dual-arm telerobotic manipulators used by the Department of Energy for decommissioning and decontaminating nuclear reactors.

Simulation Study of Adaptive Controllers for Wheeled Mobile Robots. JENNIFER ANDREWS (*University of Virginia, Charlottesville, VA 22904*) WARREN DIXON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

In this project, the performance of a recently developed modular adaptive controller was examined that enables wheeled mobile robots (WMRs) to track a time varying reference trajectory despite parametric uncertainty associated with inertia and friction. The goal of this project is to demonstrate that unlike traditional control designs, the developed controller could be implemented independently of the adaptive update law, allowing improved design flexibility for both the controller and the update law. Based on the developed controller, a numerical simulation study was performed using a mathematical representation of the WMR dynamic model. To illustrate the modularity of the controller with various adaptive update laws, the controller was simulated with both a prediction error-based least-square and gradient update law. Control gains and parameter update values were determined to minimize the tracking error and the difference between the actual and desired parameter estimates. The stability of the feedback controller was also demonstrated. Improved transient/steady-state performance and modularity was then illustrated for each parameter update law. Based on the success of the simulation results, future efforts will target experimental implementation on an industrial WMR.

Assessment of Sources of Signal Variation in the PV-Reflectometer. A. CHRIS AURIEMMA (*City College of San Francisco, San Francisco, CA 94112*) BHUSHAN SOPORI (*National Renewable Energy Laboratory, Golden, CO 89401*).

The U.S. photovoltaic cells industry has sufficient production volume to warrant a move to process monitoring, but currently lacks devices appropriate for solar cells. The PV Reflectometer has the potential to provide the PV industry with fast, cost-effective, real-time process monitoring. Beta testing of the PV Reflectometer showed evidence of signal drift, which would cause inaccurate reading and greater uncertainty in comparison of results. Several factors were identified and tested for their contributions to signal variation. AC power supplies were found to be significant sources of variation and were replaced by DC supplies, which proved to be more stable. A white paper reference was also found to be a significant source of variations. Steel coated with a titanium dioxide rich paint was found to be the more stable of two alternative white references tested. Heating, both of the PV-Reflectometer's lights and of the test sample, was not found to have a significant effect on signal variation. Data on the effect of position of the test sample contradicted theoretical predictions and previously established trends, such that further testing in this area is recommended.

National Trends in the Air-tightness and Energy Efficiency of U.S. Homes. ROZY BRAR (*California State University, Fresno, Fresno, CA 93740*) JENNIFER MCWILLIAMS (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Reducing energy requirements for infiltration and ventilation of U.S. homes is of central concern to the building science community. Blower door technology is used to determine the air-tightness and air leakage of building envelopes by measuring airflow through a fan while

maintaining a constant pressure. Normalized leakage (NL), which characterizes the air-tightness of building envelopes, is calculated using fan pressurization measurements and the building geometry. Correlations between NL and housing characteristics can be found by means of statistical analysis. Comparisons between NL and floor area reveal smaller houses have greater leakage (per square foot) than larger houses. Comparison between NL and year of construction reveal houses were built tighter after the 1970s. Comparisons between NL and location reveal houses in the East North Central, West South Central, and New England regions leak more than houses in other regions. Comparisons between initial leakage and leakage reduction reveal houses with greater leakage have more potential for improvement. Further data analysis is needed to determine the effects of ducted systems on shell tightness. Data continues to be collected in order to minimize the effects of the biases within the database. The culmination of the research will be an LBL report to be published for the U.S. Department of Energy.

Mass Balance of Biomass Conversion by Gasification.

MICHELE BUZEK (University of Colorado at Boulder, Boulder, CO 80309) STEVE PHILLIPS (National Renewable Energy Laboratory, Golden, CO 89401).

The primary goal of this assignment was to perform an overall mass balance of the biomass conversion process of the Thermochemical Process Development Unit (TCPDU) at National Renewable Energy Laboratory (NREL). Before performing the mass balance, information on each of the instruments was researched. The theoretical error of each instrument was determined from the manufacturer's specifications. The total uncertainty of each measurement was calculated using the Root Sum of the Squares (RSS) method. Each of the instruments was tested and an error analysis was performed to determine the actual error associated with each instrument. The experimental results were then compared to the theoretical values. Once the errors were determined, an Excel spreadsheet was set up to calculate the mass balance. A graph was generated to show a visual representation of the mass balance with the error limits. Using Visual Basic programming language, a macro was created to automate this process. The program is designed to import the run-time data for a user-specified date from the data server and generate the mass balance spreadsheet and graph. This program can be utilized to generate a mass balance using data files from previous plant runs, as well as a mass balance for current plant runs where the program is refreshed approximately every twenty minutes, generating a near real-time mass balance.

Developing a System to Determine the Density of Aerosol Particles. LOGA CHIEFFO (Southampton College, Southampton, NY 11968) DAN IMRE (Brookhaven National Laboratory, Upton, NY 11973).

Utilizing the Single Particle Laser Ablation Time of Flight Mass Spectrometer (SPLAT-MS) and a differential mobility analyzer (DMA), a system was constructed to determine the density of aerosol particles. The system provides the aerodynamic diameter and the Stokes diameter. With these pieces of information the density of aerosol particles can be determined. Samples with a known density were run in order to calibrate the system. The calibration followed the theoretically expected values.

Study of Proton Conducting Solid Oxide Fuel Cell Electrolytes. ADAM CHRISTENSEN (Milwaukee School of Engineering, Milwaukee, WI 53202) OLGA MARINA (Pacific Northwest National Laboratory, Richland, WA 99352).

In this experiment ceramic powders, $\text{SrCe}_{0.95}\text{Y}_{0.05}\text{O}_3$ and $\text{BaCe}_{0.7}\text{Sr}_{0.2}\text{Nd}_{0.1}\text{O}_3$, were produced utilizing a combustion synthesis method. The powders were to be used for construction of a proton-conducting electrolyte for a solid oxide fuel cell. The materials produced from the combustion reaction were calcined in order to form a single-phase material. A powder X-ray diffraction method was used to verify the structure. The powders were then processed into conductivity bars that were to be measured by a four-probe voltage measuring system. The conductivity measurements were conducted in a variable atmosphere furnace as to observe the behavior of the material in either a reducing or oxidizing atmosphere.

Development of a Computer-Controlled 6-Axis Articulated Robot Arm for Nondestructive Evaluation of Complex Shapes. JOSEPH CHRISTENSEN (Moraine Valley Community College, Palos Hills, IL 60465) W.A. ELLINGSON (Argonne National Laboratory, Argonne, IL 60439).

The purpose of this project is to research the effectiveness of an articulated-arm 6-axis robot as a motion-control stage for a laser scattering system used for nondestructive evaluation of complex shapes (e.g. turbine blades). The robot-arm/laser-scattering system was tested with two flat ceramic plates. The two plates had flat-bottomed holes of different diameters drilled into them. The system was being tested to determine exactly what types of defects could be detected with the method. Present results indicate that only surface defects are being detected. The results are inconclusive regarding the detection of sub-surface defects.

Designing a Small-Scale NWTTC Drive Train for Investigation of Multiple Generator Drive Train Configurations. SERGE DELAK (Rensselaer Polytechnic Institute, Troy, NY 12180) JASON COTRELL (National Renewable Energy Laboratory, Golden, CO 89401).

Recent trends toward increasingly large wind turbines are inhibited by the disproportionate cost of high-torque drive trains that are necessary for the efficient generation of power. Multiple-generator drive trains have the potential to decrease the size and cost of wind turbine drive trains by distributing high torque among several smaller generators. Although many other advantages exist, uncertainty about power sharing remains a primary concern. As a result the National Wind Technology Center (NWTTC) is considering testing such a system on both its dynamometer, and on a small wind turbine. This paper documents the preliminary design, and component selection for such a test system. In addition to testing torque sharing among generators in a multiple-generator system, such a test bed would also be used for exploration of power electronics and permanent magnet generator configurations that could be advantageous when combined in a multiple-generator system. Additionally, replacing the drive train of the NWTTC's Unsteady Aerodynamics Experiment (UAE) turbine would provide an additional test bed for rotor and controls testing. For this reason the main specifications of this drive system were made based on the UAE turbine specifications. After considering several possible generator and power electronics configurations, a system was recommended. It is comprised of 3 Moog FAST-V4-010 servo motors to be used as generators with diode rectification to a single DC bus and a single Trace 30kVA inverter. This recommended system would cost about \$108,000 to build and has several advantages over the other configurations considered.

Feasibility Study of Rapid Duct Leakage Screening Techniques for Large Commercial Buildings. MATTHEW DUBROVICH (Lehigh University, Bethlehem, PA 18015) CRAIG WRAY (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Recent estimates indicate that fans for distributing conditioned air in large commercial buildings use as much electricity annually as approximately 10 million U.S. homes. Sometimes there is significant air leakage from the ducts, which could be 35 to 55% of the fan power requirements. Identifying and reducing such leakage would substantially improve building energy efficiency. However, in spite of recent advances to rapidly screen residential and small commercial buildings for excess duct leakage, there is no rapid means to screen large commercial buildings. The project considered several techniques, such as using energy monitoring, tracer gas pulse injections, extrapolations from branch flow sampling, and using flow hoods combined with air-handler airflow measurements. Only the latter two techniques seemed likely to meet the selection criteria: determine leakage flows to within 5% of total fan flow; one or two people could test 100 grilles in 2 hours or less; and use only simple, commercially-available equipment. Preliminary field tests indicate that sampling is not feasible due to variations between supply grille flows and the inaccuracy of the manufacturer-installed terminal-box flow-measurement devices. In contrast, using commercially-available flow hoods appears promising: one of the five hoods tested has an accuracy better than 3% and a pair of such hoods could be used to measure 100 grilles in less than 2 hours. However, the air-handler flow-measurement device tested only had an accuracy of about 5%, which means a more accurate method needs development for this part of the test. Further work to develop the flow hood technique should be pursued.

Finite Element Analysis of the Berkeley Town House's Response to Seismic Activity. LAMONT DUKES (Evergreen Valley College, San Jose, CA 95135) DEBORAH HOPKINS (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Finite-Element Analysis was used to acquire a better understanding of building response to seismic loads. This work is part of a larger project in which the overall goal is to instrument a building with new wireless-sensor technology. The sensors will monitor the structure's acceleration and communicate that information to a server. The networked sensors are lightweight, low cost, and low power. The location of the sensors is of utmost importance to accurately measure local building accelerations. One of the objectives of the finite-element analysis is to help identify the best placement of sensors. Results of the analysis will also be used to study the building's response to seismic loads, and to help determine earthquake retrofit strategies. The Finite-Element technique is a linear, static and dynamic problem solver. ANSYS, an industry standard, numerical approximation computer program was the platform used for the simulation model development. The program has the capability to perform structural analysis, more specifically, modal and spectrum analyses: Modal analysis consists of calculating natural frequencies and corresponding mode shapes. Spectrum analysis shows peak displacement, velocity, or acceleration versus frequency. These analyses provide valuable insight into structural behavior in response to seismic motion.

Spectroscopic Exploration of Spark Plug Erosion. CARL ENG (Suffolk County Community College, Selden, NY 11784) JOHN WHEALTON (Oak Ridge National Laboratory, Oak Ridge, TN 37831). Although much research is being done in alternative fuel engines, room still exists to develop technologies in gasoline internal combustion engines to make them more efficient and cleaner. One such avenue of development is the process of spark ignition from a spark plug. A stainless steel pressure chamber was created to accommodate a variety of spark plugs. The light from the spark, observable from a quartz window on one end of the pressure chamber, is carefully focused through a series of lenses into a fiber optic cable that transmits the light to a spectrometer. Connecting directly to the spectrometer is a Charge Injection Device (CID) camera that records the spectrum lines to a computer. It will be shown that analysis of the data collected may be used to determine the rate of erosion per spark event for a spark plug, through the determination of the ratio between surface specific and volumetric spectrum lines. Furthermore, the failure of the ceramic dielectric around the center electrode, resulting in a leakage of voltage prior to the breakdown phase of a spark, will be studied on plugs of varying age and may correlate the erosion study results. The utility of the apparatus will be shown in the testing of spark plugs for an alternative fuel engine that uses natural gas. The results of this study have the potential to be highly beneficial to the automotive industry in that it will provide an economical and effective means of testing and developing spark plugs.

Assessment of the Development Process Producing the Cathode Component Within Solid Oxide Fuel Cells. JENNIFER ETTER (Villanova University, Philadelphia, PA 19085) TERRY CRUSE (Argonne National Laboratory, Argonne, IL 60439).

Briefly stated, fuel cells generate electrical energy by electrochemically combining fuel and oxidant gases across an ionic conducting aide. This method increases efficiency while decreasing harmful byproducts. Solid oxide fuel cells are fuel cells containing a solid oxide electrolyte, surrounded by the standard anode and cathode materials, and connected to additional fuel cells by interconnects. Interconnects are responsible for providing the electronic connection between the fuel cells, which builds voltage. Each component of the cell must have the proper stability in oxidizing and/or reducing environments, chemical compatibility with other components, proper conductivity, and similar coefficients of thermal expansion to avoid cracking during fabrication and operation. However, each component has unique responsibilities in the energy conversion process, and must meet different requirements. Cathodes need to contain a porous microstructure to allow gas transport to the reaction sites as well as high catalytic activity. They are tested using a half-cell electrochemical test apparatus, which omits graphs illustrating the impedance allowing ohmic resistance to be obtained, as well as the electrode/interfacial resistance. An electrode/interfacial resistance of 0.1 ohm is considered optimal.

Phase Noise Characterization of the Main Drive Line at SLAC. DREW FUSTIN (Drake University, Des Moines, IA 50311) RON AKRE (Stanford Linear Accelerator Center, Stanford, CA 94025).

The phase noise of the Main Drive Line (MDL) at the Stanford Linear Accelerator Center is extremely important to the operation of the linac since the MDL provides the radio frequency (RF) drive and phase reference for the entire accelerator system. In order to ensure that the Linac Coherent Light Source (LCLS) can be run using current MDL components, the phase noise of the MDL had to be ascertained. This was determined using an ultra-stable reference oscillator phase-locked to the MDL. Using this device, the phase noise was determined to be far greater than LCLS requires. This suggests that an improved Master Oscillator needs to be obtained in order to be able to run LCLS on the SLAC linac.

Electrostatic Trapping and Detection of Photosystem I Molecules. BRENT GEORGE (Tennessee Technological University, Cookeville, TN 38501) JAMES LEE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Testing the electrical transport characteristics of single molecules can be difficult. Fortunately, there is a technique to overcome this problem. The technique is called electrostatic trapping. This technique uses nano-scale electrodes in an open circuit configuration. The gap of the open circuit is left slightly smaller than the molecule one wishes to test. A potential is applied across the gap to electrostatically attract a single molecule between it. The single molecule will become trapped between the electrodes and its V-I characteristics can then be measured. The process first starts with an n-type 100 silicon wafer. Next silicon oxide is grown on top as an insulation layer. Next, the wafer is coated with PMMA photo resist and e-beam lithography is used to imprint a pattern into the PMMA. After this, the wafer is immersed in developer for two minutes and dried with nitrogen. Then, the wafer is coated in 5nm of chromium and 50nm of gold. Next, the sample is immersed in acetone for 2-4 hours and the unwanted gold is released from the structure. This leaves a fully released nano-structure with a gap spacing of about 20-50nm. Lastly, the tip of one electrode is platinized to shorten the gap spacing until it is approximately 4-6nm. This technique attempts to test the V-I characteristics of the Photosystem I molecule.

Seismic Analysis of TPS Conduit Mounts. BOBBY GOINS (Mississippi State Technical Community College, Knoxville, TN 37933) RON BATTLE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Seismic Analysis of TPS Conduit Mounts Conduit mounts were designed for the Spallation Neutron Source (SNS) target safety and nonsafety class control and protection systems. The mounts for conduit that carries safety class cables have specific seismic requirements placed upon them because they are part of the Target Protection System (TPS) that ensures protection of the public from potential target accidents. The conduit mounts for the TPS, a safety class system, were analyzed to guarantee that the cables contained within the conduit would not be damaged during a seismic event. The method used to analyze the mounts included calculating the maximum possible seismic load that could be applied to the mounts then comparing that load with the allowable working load determined by vendor tests. The nonsafety conduits protect instruments inside the target utility vaults and route the cables to cabinets and instrument racks located outside the radiation area. The results of the seismic analysis done on the TPS conduit mounts, which was documented in a draft report, confirmed that each of the mounts would withstand a seismic event. The final designs were given to a contractor for installation in the SNS Front-End Building and klystron gallery and will also be given to the cable installation contractor for installation in other SNS buildings.

Development of TiN Coating for RF Vacuum Chambers. ALEX GRAY (Southern University, Baton Rouge, La 70807) PING HE (Brookhaven National Laboratory, Upton, NY 11973).

A thin film layer of titanium nitride (TiN) will coat the inner walls of the RF chambers for the US Spallation Neutron Source (SNS). The coating should be 100nm in thickness. The TiN coating is used to reduce the secondary electron yield (SEY) that will occur inside the chamber due to the proton particle acceleration, thus making the chamber, in a sense, wear resistance. The TiN coating will be evaluated by its surface properties, color dispersion, element content, and oxidation behavior.

Creating a Custom Electronic Library using Orcad Capture. MICHELLE GREIGG (*Miami-Dade Community College, Miami, FL 33132*) ISTVAN NADAY (*Argonne National Laboratory, Argonne, IL 60439*).

Schematic capture is an integral part of the process of creating an electronic Printed Circuit Board (PCB). It provides the necessary link between schematic design and the creation of a PCB. Typical component libraries are a database of electronic parts that contain most of the information necessary to generate a PCB. However, they leave out the information about the component's footprint, or physical form. This information is essential to the creation of a PCB and is typically added during PCB layout and not during schematic capture. To accelerate the design process, a component library that includes the footprint information was created. This new component library created a seamless link between Orcad Capture, the schematic capture program, and Allegro Designer - the PCB layout software. These software programs are key tools in the electronic engineering design process. The new library forms the beginning of a standard set which everyone in the organization will use. The result of this work eliminates time-consuming, inefficient efforts and creates standardization. Building this library required an understanding of the complete PCB design process, learning the intricacies of Orcad Capture, and learning a significant amount about the electronic components entered into the database. This work is an ongoing process because of the enormous number of parts and because new components emerge daily.

Variable-Air-Volume Box Performance. JEFFREY GUASTO (*Lehigh University, Bethlehem, PA 18015*) NANCE MATSON (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The purpose of this study was to determine the thermal efficiency of parallel-fan-powered pressure-independent variable-air-volume (VAV) boxes, as part of a larger research project to characterize thermal distribution system performance in large commercial buildings. These types of VAV boxes control the flow rate and temperature of conditioned air supplied to occupied spaces by mixing pre-conditioned primary air with induction air from the ceiling return air plenum; temperature is also controlled using auxiliary reheat from an integrated electric heater or hot water coil. The ability of these VAV boxes to deliver the entire box input energy to downstream ducts without losses was unknown to both manufacturers and researchers. In this project, a new thermal efficiency parameter that accounts for the VAV box energy balance was developed based on heat transfer, thermodynamic, and fluid mechanics theory. Using this theory and data acquired from two sample VAV boxes, the instantaneous and cumulative thermal efficiency was calculated for operating hours during typical winter (heating) and summer (cooling) days. Efficiencies were near 100% except in the heating mode, where the instantaneous efficiency of the VAV box dropped to as low as 40% when the heater was fully energized; the cumulative efficiency was much higher (about 80%), because the heater does not always operate. Further study is needed to define and understand the heater-related loss mechanisms.

Surface Stress Measurements in Automotive Glass.

ANTHONY GUZMAN (*Columbia Basin College, Pasco, WA 99301*) KENNETH I. JOHNSON (*Pacific Northwest National Laboratory, Richland, WA 99352*).

This research focuses on the measurement of residual stresses in automotive side windows. Residual stresses are the stresses that occur after the glass has been formed. Stresses were measured in three glass samples: 1) a 3.8 mm thick, 304.8 mm x 304.8 mm (12x12 inch) laminated flat test specimen, 2) a 4.7 mm thick 304.8 mm x 304.8 mm laminated flat test specimen, and 3) a fully laminated side window measuring 4.7 mm in thickness. The surface residual stresses were measured using a grazing angle surface polarimeter (GASP). This tool utilizes birefringence introduced by residual stress in the tempered glass as the measurement parameter. Birefringence is the splitting of a ray into two parallel rays polarized perpendicularly. The birefringence is directly proportional to the magnitude of the stress differences. The stress measurements were taken in three orientations (0, -45, +45 degrees) and transformed into maximum and minimum principal stresses using a Mohr's circle approach. The principal stresses were then plotted using the ANSYS finite element code to obtain smooth contour plots. The principal stresses provide baseline stresses in the development of a finite element model, which will be used to estimate the stress distribution in side windows during door-slam loading. The purpose of this study is to correlate results and actual door slam tests

with measured glass strength data. This project is beneficial to the Department of Energy (DOE) because its main purpose is to reduce weight and fuel consumption in automobiles.

Development of an Automated Microfluidic System for DNA Collection, Amplification, and Detection of Pathogens.

BETHANY HAGAN (*Washington State University, Pullman, WA 99163*) CYNTHIA BRUCKNER-LEA (*Pacific Northwest National Laboratory, Richland, WA 99352*).

This project was focused on developing and testing automated routines for a microfluidic Pathogen Detection System. The basic pathogen detection routine has three primary components; cell concentration, DNA amplification, and pathogen detection. Cell concentration is achieved by using magnetic beads that are held in a flow cell by an electromagnet. Sample liquid is passed through the flow cell and bacterial cells attach to the beads. These beads are then released into a small volume of fluid and delivered to the peltier device for cell lysis and DNA amplification. The cells are lysed during initial heating in the peltier device, and the released DNA is amplified using polymerase chain reaction (PCR). Once amplified, the DNA is then delivered to a laser induced fluorescence detection unit in which the sample is detected. These components combined create a flexible platform that can be used for pathogen detection in liquids derived from environmental samples such as water, sediments or aerosols. Future developments of the system will include on-line DNA detection during DNA amplification and improved protocols to minimize the analysis time and minimize the use of reagents.

Multiple Biometric Sensors Working on an Integrated Platform. MEIR HERSHCOVITCH (*Massachusetts Institute of Technology, Cambridge, MA 02139*) UPRENDRA ROHATGI (*Brookhaven National Laboratory, Upton, NY 11973*).

The use of biometric security systems are quickly becoming commonplace in many industries. However, as with any new technology, there are flaws and errors. Our goal is to create an integrated biometric security system that utilizes many devices such as fingerprint identification, hand recognition, voice recognition and face recognition. All of these devices have a small error rate working alone, however; working in unison their error rate decreases significantly. We took these four biometric devices and tried to make them work with our own code. It was necessary to purchase a fingerprint scanner from the market and then try to make it work on our own software. We built our hand recognition device. We also purchased a camera and a microphone for the face and voice recognition programs. After the devices were purchased or constructed, it was necessary to make them work on our own pieces of software. The advantage of programming our own software for each device is that later on it will be easier to integrate the 4 programs to work as one. The programming was done in Visual C++. So far we were able to get our software working with all the devices individually and are currently working on integrating all of them to work as one unit. Once this happens, it will hopefully revolutionize the sale of biometric security devices. It will hopefully convince companies to invest in not one, but a combination of biometric security devices which would now be available in one unit. This device would also make false identification far less common.

Rapid and Remote Prototyping of Direct Sequence Spread Spectrum Radio Frequency Transceiver Designs. BENJAMIN HUEY (*Pellissippi State Technical Community College, Knoxville, TN 37933*) PAUL EWING (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The RF & Microwave Systems Group at Oak Ridge National Laboratory builds many transceiver prototypes for a wide range of applications. It costs the group a great deal of time and money to create new prototypes for each project. The problem is now being solved by using a system of modular radio frequency circuit boards and a vector signal analyzer. Each component in the system is remote programmable through a LAN connection and has the capability of connection to the Internet. This allows users to quickly create a prototype for a given problem from any location with access to the Internet and view an analysis of the signals being produced. This system is a cost effective alternative to building single use prototypes for individual projects.

Finite Element Modeling and Analysis of the Berkeley Town House. FAI JOR (*Evergreen Valley College, San Jose, CA 95135*) DEBORAH HOPKINS (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Finite Element (FE) modeling is good way to predict the seismic response of buildings. A model is created by dividing the building into many smaller pieces and generates a series of equations to calculate the solutions. It can give results very quickly with the help of computer. For this project, FE analyses are performed in a computer program called ANSYS. The first few tasks are to get some background structural-engineering information and to retrieve some key information about the building such as building materials and dimensions. After that, creation of keypoints, lines, and areas based on the dimensions of the building is done to represent the columns and shear walls of building. Meshing is the procedure to make the model into a few thousands of smaller pieces to perform calculations. Modal and spectrum analyses are done to find out the natural frequencies, deformed shapes, and stress concentration of the building. Results of modal analysis show that the building either bends or twists during an earthquake. Spectrum analysis shows that the top of the building has the greatest motion during earthquake while the bottom of the building suffers the greatest stress. The results of the analyses can help to determine the best locations of accelerometers. They also help to determine which parts of the building should be retrofitted.

Laser Profile Tracking of Small Animals in SPECT Imaging.

RYAN KEREKES (*University of Tennessee Knoxville, Knoxville, TN 37916*) SHAUN GLEASON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Recent studies of the mouse genome have shown that laboratory mice are extremely valuable tools for modeling human disorders. Such models have allowed scientists to better understand the origins of disease and develop new treatments to counteract them. High-resolution Single Photon Emission Computed Tomography (SPECT) and X-ray Computed Tomography (CT) imaging have proven to be useful techniques for non-invasively monitoring mutations and disease progression in small animals. A need to perform in vivo studies has led to the development of a small-animal imaging system that integrates SPECT imaging equipment with a pose-tracking system. The pose of the animal is monitored and recorded during the SPECT scan using either laser-generated surfaces or infrared-reflective markers affixed to the animal. The laser-based system uses a pair of high-speed scanning lasers and CCD cameras to acquire a series of 3-D images of the surface of the animal. The acquired surfaces can then be registered to a reference surface to determine the relative pose of the live animal and correct for any movement during the scan. The surfaces can also be used for registration of the SPECT and CT data sets for functional and anatomic image registration.

Fabrication and Characterization of Vertically-Aligned-Carbon-Nanofiber-Based Membrane Devices. KATE KLEIN (*Trinity College, Hartford, CT 06106*) MICHAEL GUILLORN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Materials with nano-scale features have the potential for widespread use in biomedical applications. Nanostructures like vertically aligned carbon nanofibers (VACNFs) can be incorporated into devices in order to mimic natural systems. The goal of this research was to fabricate and characterize microfluidic channels containing stripes of VACNFs, which act as diffusion barriers or "membranes". These membrane devices control the transport of materials across a synthetic barrier. The VACNFs were prepared by a catalytically controlled plasma enhanced chemical vapor deposition (PECVD) process that provides for their directed assembly. Conformal coating with PECVD silicon dioxide modified the interfiber spacing or "pore size" of the membrane. Four methods of producing the microfluidic channels integrated with VACNF membranes were investigated in this study. The fiber and channel structures were characterized using a scanning electron microscope (SEM). The transport properties of fluorescently labeled latex beads flown through VACNF membranes were observed using a fluorescence microscope. The fluorescent beads were transported through the device either by means of simple diffusion, electro osmotic pumping, or a hydrostatically driven Nanoport® syringe-pump assembly. Results show that the VACNF barriers promote the size separation of latex beads (50-750 nm) corresponding to the pore size of the membrane. The results also suggest that by altering the VACNF interfiber spacing or array density, the properties of the membrane can

be adjusted. These types of membranes may be useful for molecular sorting and mimicking the transport properties of natural membranes.

Modeling of a Small-Scale Ammonia-Water Absorption Cooling System. JOEL LINDSTROM (*Montana State University, Bozeman, MT 59715*) BOB WEGENG (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The objective of this assignment is to generate a simulation model for a single stage, ammonia-water ($\text{NH}_3\text{-H}_2\text{O}$) absorption cooling system, relevant to small-scale (150 W) applications. To date, Lithium Bromide-water ($\text{LiBr-H}_2\text{O}$) absorption systems have been used, however, the high vapor pressure of ammonia could lead to a smaller, lighter, more compact cooling system. Many parameters require evaluation in the design of an absorption cooling cycle. The model under development offers quick simulation and interpretation when changing one or more of its operating parameters. A developmental program, Absorption Simulation (ABSIM), is used to facilitate this model. After the first stage of modeling, it is concluded that it is necessary to provide a means to extract undesirable water from the ammonia in the refrigeration loop, especially when the heat rejection temperature (atmospheric air) could be as high as 45°C. A solution to this problem may be to add a reflux cooler or rectifier, or at the very least add a mechanism capable of draining liquid water from the evaporator. A very important output of simulation, the work done by the working fluid pump, is anticipated to be on the order of 85 W given a cooling duty of 150 W.

Pursuing the Prototype of a New Generation of Radiation Area Monitors. VIR ANGELO LONTOC (*Essex County College, Newark, NJ 07107*) VINCENT J. CASTILLO (*Brookhaven National Laboratory, Upton, NY 11973*).

The radiation area monitors, commonly referred to as "chipmunks", that are currently used at the Collider-Accelerator (C-A) Complex at Brookhaven National Laboratory was designed more than two decades ago. This has led to the project of upgrading the design of the chipmunk. All aspects of the existing chipmunk, including the power supply, circuit components, sub-circuitry, and electronic packaging are being critically reviewed for modernization.

Two Dimensional X-Ray Detector Design. NICHOLAS LYNCH (*Lehigh University, Bethlehem, PA 18015*) GEORGE MAHLER (*Brookhaven National Laboratory, Upton, NY 11973*).

The two-dimensional x-ray detector has the capability of pinpointing the vertical and horizontal position of an incident x-ray. It can then feed the information to a computer that can create an image displaying the position and frequency of the x-rays. The National Spherical Torus Experiment at the Princeton Plasma Physics Laboratory requires such a device to study the plasma formed during nuclear fusion reactions. The detector consists of an argon or krypton gas chamber and a set of anode wires stretched perpendicularly across a set of cathode strips. The x-rays are absorbed by the gas and the resulting ionization collects across the anode and cathode. Based upon the horizontal and vertical positioning of the collected charges, and image can be formed displaying the location and intensity of the incident x-rays. Their application requires a detector with a particularly large viewing for low energy x-rays. These requirements create a set of design complications that must be overcome. Challenges include designing a support structure for the beryllium window, designing both the anode and cathode plates, and developing a gas chamber free of leaks.

Design and Cost Analysis of New Inlet Section of the Supercritical Carbon Dioxide Test Loop. HEATHER MCCAIG (*Oregon State University, Corvallis, OR 97331*) FADEL ERIAN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The inlet section of the supercritical carbon dioxide test loop at Pacific Northwest National Laboratory was redesigned. The original inlet design allowed for flashing of liquid CO_2 , causing icing of the piping system preventing the high pressure LEWA pump from being primed. The new design incorporates a liquid CO_2 supply tank, a chiller, and a heat exchanger. The new design was made along with the operational procedures for charging the inlet section. The thermodynamic path of the inlet was also included. The chiller and heat exchanger were sized and price quotes were obtained for each. A cost analysis was done on the redesign of the inlet.

Investigation of the Stability of the RF Gun of the SSRL Injector System. JESSICA MOORE (*Loyola Marymount University, Los Angeles, CA 90045*) BENJAMIN SCOTT (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

In the previous three years, Stanford Synchrotron Radiation Laboratory (SSRL) has experienced electron beam instabilities in the injector system of the Stanford Positron Electron Asymmetric Ring (SPEAR). Currently, for approximately the past four months the radio frequency (RF) gun of the linear accelerator injector system of the SPEAR at SSRL has become increasingly unstable. The current of the RF gun has become progressively sluggish and the lifetime of the cathode within the RF gun has been much shorter than expected. The cathode also sustains many unexplained damages. The instability of the RF gun affects the entire operation of SPEAR, creating substantial inconvenience. Through mechanical, design, and procedural analysis of the RF gun and the cathode that emits the electron beam of the linear accelerator, a solution to prolong the life of the cathode and secure the stability of the gun can be found. The thorough analysis of the gun and cathode involves investigation into the history of cathode installation and removal through the years of SPEAR operation as well as interviews with SSRL personnel involved with the upkeep of the gun and cathode. From speaking with SSRL employees and reviewing several articles many possible causes for beam instability were presented. The most likely cause of the SSRL gun instability is excessive back bombardment that can be attributed to running the cathode at too high a temperature.

Growth of Carbon Nanotubes by Chemical Vapor Deposition (CVD). NERY MORENO (*East Los Angeles College, Monterey Park, CA 90220*) PATRICK GAMMAN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Carbon nanotubes have been studied with great interest because of their remarkable electronic, mechanical, and electron field emission properties. Our research mainly dealt with the growth of carbon nanotubes by chemical vapor deposition (CVD) and the study of their electron emission properties. Carbon nanotube growth by CVD uses a hydrocarbon gas and decomposes it on a transition metal catalyst, usually Fe, Ni or Co. Carbon nanotubes are grown on a heated catalytic quartz substrate by means of acetylene pyrolysis. Their growth is dependent on several variables, such as tank pressure, substrate temperature, catalyst used, and $C_2H_2:NH_3$ ratio in the N_2 submerged tank. The C_2H_2 is what triggers carbon nanotube growth and the NH_3 prevents an unwanted carbon film from forming on the entire substrate. Because of the electron field emission properties that carbon nanotubes possess, our group's major goal is to use a thin ring of carbon nanotubes as an efficient, powerful electron source for an electron disc accelerator. To test for electron field emissions, a bell jar vacuum system was used. Although this system does not allow for electron emission to be viewed, photon emissions are visible and therefore since photon emission are dependent on electron emission, one can conclude that electron emissions must be present.

Biofluidization Modeling: What is Available and What is Needed? PASCHALIA MOUNTZIARIS (*Princeton University, Princeton, NJ 08544*) SREEKANTH PANNALA (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Biological fluidized bed reactors (FBR's) were developed in the early 1970's and were mainly used to denitrify wastewater. Due to their compact size and increased efficiency, these reactors gained popularity in many industries, with current applications ranging from treatment of industrial wastewater to simulation of human tissue. The main problems with biological FBR's are the mechanical scale-up of the influent distribution system and the lack of economically attractive commercial systems. To identify feasible solutions, researchers have been working on creating accurate models of these reactors. A commonly used "test-bed" for developing the multiphase flow equations that describe FBR's is called MFIx (Multiphase Flow with Interphase eXchanges). MFIx is a general-purpose computer code developed at the National Energy Technology Laboratory (NETL) for describing the hydrodynamics, heat transfer, and chemical reactions in fluid-solids systems, based on a generally accepted set of multiphase flow equations. This paper addresses the use of MFIx and discusses modifications that need to be made to expand its range of applications (e.g. bubbling and circulating fluidized beds). The most significant change focuses on extending its current two-phase capability to three phases. Other modifications include the development of equations to

simulate poisoning of the microorganisms due to high concentrations of pollutants and eventual erosion of the substrate on which the microorganisms are growing. The extension of this powerful code to modeling the phenomena associated with biofluidization would facilitate not only the improvement of biological FBR's, but of FBR's in general.

Analyzing Transitional Flows Adjacent To Compliant Surfaces With A Spectral Element Code. LATEEF MUHAMMAD (*Chicago State University, Chicago, IL 60628*) PAUL FISCHER (*Argonne National Laboratory, Argonne, IL 60439*).

Wall vibration has been postulated as a possible energy dissipation mechanism in transitional flows adjacent to compliant surfaces. The capability to investigate such combined fluid-structure interactions in a spectral element code is further developed for fluid-structure interaction problems. We present cases simulated of compliant wall interaction with transitional flows: a shaped free surface, a sinusoidal wall changing shape or moving.

Data Simulation for Mica Mote Networks. MATTHEW NIELSEN (*Ripon College, Ripon, WI 54971*). DEBORAH L. HOPKINS (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Emerging wireless-sensor technology has promise for many real-world applications. Developing the proper software tools to operate a network of these sensors involves such tasks as calibration, eliminating noise, recognizing problems in the network, developing a communications protocol, network and sensor management, and translating data into meaningful values. Data translation is a necessary first step in attempting to comprehend the nature of the sensors. Scenarios were created in order to model simulated data with superimposed noise under realistic conditions. These scenarios centered on a real-world application involving a building occupancy detection model, allowing rescue workers to know how many people are located in particular sections of a building during a catastrophe. The sensors we use are called mica motes, and come equipped with a thermistor, an accelerometer, a magnetometer, a photo sensor, and an acoustic sensor. Radio frequency boards attached on both the sensors and the computer provide communication throughout the network. Once proper software has been developed for these sensor networks, they will have a variety of applications, including improving building energy management, monitoring manufacturing processes, assisting with inventory management, and environmental monitoring.

Design of a Printed Circuit Board for the 5-Channel Noise Reduction/Isolation Circuit. OLUSOLA OLAODE (*Monroe Community College, Rochester, NY 14623*) OMAR L. GOULD (*Brookhaven National Laboratory, Upton, NY 11973*).

A printed circuit board is designed for an electronic circuit that provides increased noise immunity and electrical isolation of signals. An existing electrical schematic of a circuit that provides increased noise immunity and electrical isolation is modified from providing two signal channels to providing five signal channels. Noise can cause false triggering in electronic logic circuits. The purpose of the electronic circuit is to increase the noise immunity of the beam request signals entering the Linear Accelerator (LINAC) Timing System located in the LINAC control room. The original circuit was designed on a prototyping card with pre-drilled pads and wire connections. The noise immunity of the new electronic circuit is improved by the printed circuit board design. The 5-channel noise reduction and isolation circuit is to be mounted in an enclosure and installed into a 19" x 8.5" x 10" maximum rack space. The PC board layout was designed using Protel 99Se software and constructed with ProtoMat 92S manufactured by LPKF Laser & Electronics.

Computational Model of Mechanical Wall Stress in a Human Abdominal Aortic Aneurysm One-Hour Prior to Rupture. JOEL OUTTEN (*University of Tennessee Knoxville, Knoxville, TN 37922*) KARA L. KRUSE (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

There has recently been much research aimed at modeling human abdominal aortic aneurysms (AAA) utilizing computed tomography (CT) scans and finite element analysis. However, the theoretical rupture sites generated by previous modeling efforts have yet to be verified, due to the fact that rupture generally does not occur immediately after CT scan acquisition. A unique case study, in which a patient experienced AAA rupture approximately one hour after CT scans were

acquired, has been undertaken. Commercial software was utilized to first establish a method for creating a geometry model for the human AAA from CT scan images. A finite element model of the aneurysm was then constructed and used to determine the optimal parameters for obtaining efficient and reasonable stress results. A static intraluminal pressure, simulating an average blood pressure, was applied to the model. En route to obtaining the final calculations, this model was also used to compare recently published hyperelastic parameters with traditional elastic AAA conditions in an effort to determine whether or not one model proved to more accurately predict rupture location. The resulting highest realistic stress occurred on the anterior side of the aneurysm, distal to the bulge. Both the hyperelastic and the linear elastic model gave the same maximum stress location, with similar stress distributions elsewhere. The model will soon be compared with the actual clinical system in order to verify the model's validity.

Portable Biochip Reader. DAN PATES (*Kirkwood Community College, Cedar Rapids, IA 52404*) GENNADIY YERSHOV (*Argonne National Laboratory, Argonne, IL 60439*).

Biochips developed at Argonne National Laboratory (ANL) are glass slides that are prepared so they have arrays of small gel-pads on their surface. These gel-pads act as test tubes to hold oligonucleotide probes. When sample DNA hybridizes to target DNA in the gel-pads they will fluoresce when excited by laser light. My project involved building a portable reader that reads the fluorescent intensity from the gel-pads. The Biochips must be read to ensure they were made properly and also to analyze the DNA of the sample. The reader developed at ANL has many advantages over commercially available readers. It is small, portable, faster, and far less expensive. My lab partner and I gathered the parts, assembled them, and made the proper alignment of the optical components. The alignment of the optical pathway was paramount. It must be precise to only a few hundred microns in order to get the proper view of the gel-pad surface and proper readings of the fluorescent intensities. The readings from the two Biochip readers that were built were compared using calibration slides. One of the readers showed the expected intensities after assembly, and the other functioned properly but indicated lower intensities than the others. This problem was traced to the laser sources. The readers are currently being tested by outside evaluators in preparation for commercialization.

Web Base Electrometer Monitoring and Controlling Using Infrared Decoding Microcontrollers. CARLOS PENA (*State University of New York at Stony Brook, Stony Brook, NY 11794*) ANTHONY KUCZEWSKI (*Brookhaven National Laboratory, Upton, NY 11973*).

There are many detectors requiring electrometers used at Brookhaven's National Synchrotron Light Source (NSLS); most of the instruments are made by Keithley Instruments Inc. The objective is to allow for a much more inexpensive and convenient approach to beamline detection as well as noise reduction for user-operated beamlines when obsolete units need replacing. Commonly used for ion chambers and Passivated Implanted Planar Silicon (PIPS) detectors, this in-house designed operational-amplifier electrometer is connected to an embedded computer to allow for remote control accessibility. The variable gain electrometer (switchable from a gain of 105 to 1010 Volts/Ampere [V/A]) will respond to infrared (IR) commands decoded by a Programmable Interface Controller (PIC)16C54C microcontroller sent from an uCdim Dragon Ball VZ microcontroller (MCU) using Panasonic's LN54 GaAs infrared Light Emitting Diode (LED). The communications between these microcontrollers is through a Pulse Width Modulated (PWM) IR signal with a 38kHz carrier frequency. Encoded in the pulse width modulated signal are preparatory pulses followed by an 8-bit word commonly used in consumer electronics. The transmitted signal is received by Panasonic's PNA4612M Series Photo Integrated Circuit infrared receiver demodulator and is decoded using the PIC16C54C into an address and a command for the electrometer. Each electrometer has its own address and references the received address to determine whether the received command corresponds to that particular electrometer. The resulting web electrometer will provide an economical alternative for user-operated beamlines when they need to replace obsolete units.

Conversion of NSLS Accelerator Ring Survey Data into Global Coordinates. JAVIER PEREZ (*Universidad de Puerto Rico, Río Piedras, PR 00931*) and CHARIS WALKER (*Saint Augustine's College, Raleigh, NC 27610*) EDWUIN HAAS (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

The National Synchrotron Light Source (NSLS) operates two electron rings: an X-Ray Ring and a Vacuum Ultraviolet (VUV) ring. Both provide intense, focused light in different wavelength regions for scientific experiments. As part of the Mechanical Section at NSLS, surveyors align and monitor the position of any of the dipole magnets and beamline components. A small shift in the position of any of the dipole magnets would alter the positions of the orbiting operation. Positional data taken in local coordinates was compiled over the past several years, but was never converted into global coordinates and never compared from year-to-year to determine if structural settling or shifting of magnet positions has occurred. Commercially available STAR*NET software was used to help automate the data processing and conversion of survey data into global coordinates. However, in order to understand and validate the data processing, manual data calculations were performed extensively. Trial-and-error of many different mathematical methods was used since source code was not provided. Using manual calculations, fairly close agreement with the computer calculations was obtained. The mathematics and data processing both posed many challenges due to the amount of data and the limited time to: determine the mathematics used, check the calculations manually, learn how to use the STAR*NET software, the process, and interpret the data.

HANDSS-55. SAMUEL PETERSON (*Brigham Young University, Provo, UT 84604*) ROD SHURLIFF (*Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID 83415*).

DOE facilities around the nation have in their possession low-level nuclear waste or transuranic waste (TRU-waste). This TRU-waste is stored in thousands of 55-gallon drums. DOE facilities have been or are going to store TRU-waste into the Waste Isolation Pilot Plant (WIPP), an underground repository licensed to safely and permanently dispose of transuranic radioactive waste left from the research and production of nuclear weapons. To prepare 55-gallon drums of TRU-waste manually is dangerous, timely, and costly. The Handling and Segregating System for 55-gallon Drums (HANDSS-55) provides an automated technology to process TRU-waste and mixed TRU-waste. HANDSS-55 opens 55-gallon drums and liners and prepares the waste inside these drums for shipment to WIPP. The technology incorporated in the HANDSS-55 is both automated and modular, allowing individual modules to be used with a multitude of other applications. The HANDSS-55 system performs four main processes: Automated Drum and Liner Opening (AD&LO), Process Waste Reduction (PWR), Waste Sorting, and TRU-Waste Repackaging. The system is still being developed and has not reached final stages. The AD&LO has been completed and tested very well. Testing on other sub-systems have also been done and led to many changes and enhancements, due to errors that occurred. Nevertheless, HANDSS-55 will play an important part of sorting and repackaging nuclear waste for the future.

The Design and Development of Proton Beam Dump Temperature Monitoring System. LAV ROHATGI (*Indian Institute of Technology Kanpur, India, Kanpur, India, UP 208016*) BRIAN OERTER (*Brookhaven National Laboratory, Upton, NY 11973*).

For any system to function properly it is necessary to maintain a temperature within a fixed range. Similarly the proton beam dump system in the Spallation Neutron Source in Oak Ridge National Laboratory, Tennessee, also works within a fixed temperature range. So it becomes important to devise a fail proof method of monitoring and controlling the temperature of this system. In order to monitor and control the temperature 28 thermocouples have been employed which are controlled by a Programmable Logic Controller (PLC). This PLC sends the temperature over the Local Area Network (LAN) to a front-end computer from where the data can be accessed and monitored and the alarm thresholds can be changed. If this threshold is exceeded the whole system is made to shut down. This system when implemented will protect the proton beam dump system and will also increase the safety of the system by shutting it down in case of overheating.

The Goes Over All Terrain Vehicle. TRENT ROTH (*Bismarck State College, Bismarck, ND 58501*) MICHAEL W. RINKER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The demand for robots to be involved in extended military missions, national defense, and homeland security is increasing. The Goes Over All Terrain Vehicle (GOAT) was designed to meet the requirements of a joint project between the Defense Advanced Research Projects Agency (DARPA) and the United States Army called the Future Combat Systems (FCS). The FCS was looking for an Unmanned Ground Combat Vehicle (UGCV) to utilize the state of the art robotic technology to minimize ground crew involvement. During the first phase of the DARPA project, Pacific Northwest National Laboratory (PNNL) completed the design of a prototype GOAT vehicle. The FCS project chose to deploy much sooner than initially estimated and the innovative concepts, like GOAT, were not chosen in a down selection for the second phase of the project. However, DARPA did allow PNNL to use the remaining funds to build a proof of concept vehicle. With a minimal budget, the prototype GOAT has emerged from a design on the computer. Preliminary tests show that GOAT has had minor hardware problems and suffered setbacks due to the limited budget. However, it will be an extremely viable candidate for the technological advancement of autonomy in robots.

Evaluation of FEMLAB as a Magnetic Field Modeler. CORY RUPP (*Montana State University, Bozeman, MT 59715*) RONALD HATCHER (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

Numerical modeling is a powerful tool for solving complex problems. A numerical code called FEMLAB utilizes this and Finite Element Analysis (FEA) to solve real world problems that would otherwise need to be solved experimentally. Before it is used however it must be checked on simple problems for solution accuracy and simplification applicability. These are done to verify that the program will give correct results on more complex models such as the toroidal field coils of the Next Step Spherical Torus (NSST). FEMLAB will also be used to optimize the shape of the coils on NSST, which will enable better performance of the experimental device.

Biolistic Gene Gun. JONATHAN SIEGRIST (*University of California Los Angeles, Los Angeles, CA 90024*) JIAN JIN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Biolistics is a method of transfection involving the firing of DNA coated micro-particles into a specimen. Currently, the most widely used method of transfection involves injection of DNA into a specimen using a needle, often resulting in over doses of DNA and damage to the specimen. Biolistics provides an alternative to this transfection technique, and has been used successfully in the past. In this approach, the metal particles, or microcarriers, are coated with DNA and fired into the specimen using compressed gas. Current biolistic devices have many limitations, including the inability to deliver particles to a small, pre-selected area. Having a small target area would enable transfection of small and even microscopic specimens. An organism whose use in genetic studies is becoming widespread is a roundworm in the Nematoda phylum named *Caenorhabditis elegans* (*C. elegans*). A single worm is only 1 mm long, and is therefore difficult to target. We tested three different sized apertures designed to control the blast radius. Using compressed helium to propel the microcarriers, we checked to ensure that the 1.0-micron diameter gold microcarriers passed through the apertures. We then shot *C. elegans* with each pinhole to test penetration and gene expression. We found that the microcarriers passed through each aperture and penetrated the *C. elegans* skin. Preliminary data indicated that the worms were transfected. A success rate was not determined.

Improvements to MicroCT Scanner for High Resolution X-ray Screening. THOMAS SWINDLE (*University of Tennessee, Knoxville, TN 37916*). MIKE PAULUS (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The recently developed MicroCT X-ray scanner is being updated for better functionality, safety, and quality. To prevent X-rays from escaping, a large, encompassing steel box with a system of interlocks was built and placed in a shield to further enclose the X-ray source. A single circuit board is used to integrate the hardware and software that control the equipment. The scanner uses a high-voltage X-ray source and a CCD detector that provides a resolution of 50 microns or less. A bed and rotating stage are used to position the object being scanned. Different parts and materials are being researched in order

to provide better scans and broader applications. The scanner, used primarily for screening mutagenized mice, also has applications in imaging small objects such as electronic components and various materials. The new features of this scanner have been found to increase the efficiency and the safety of X-ray research.

Automating the Control System of a Vertical Motion Apparatus to Survey Field Quality in New Superconducting Magnets.

DANIEL VALENTINE (*Christian Brothers University, Memphis, TN 38019*) RAY HAFALIA (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The purpose of this research was to find a more automated way to control the Superconducting Magnet Group's vertical motion apparatus (VMA). The VMA vertically drives a rotating probe that measures the field quality inside the bore of the prototype magnets the Superconducting Magnet Group produces and tests. The previous method was only semi-automated. Previous data acquisition was gained through the manual turning of knobs on the existing indexer and then relating the number of turns to the distance the VMA had traveled. The probe, which measures magnetic field quality, is incrementally positioned inside the bore tube of the superconducting magnet by the VMA and then data is collected from the probe at varying heights. The VMA operator stood at the indexer to jog the VMA up or down while another researcher sat at the magnet test facility control board and command the Data Acquisition System (DAQ) to record the data once the VMA operator signaled the probe was in position. During a typical magnet test run, the VMA operator positioned the probe at its start position. The researcher took the initial data point, then signals the VMA operator to go to the next prescribed position. The researcher waited until the VMA operator signaled that the probe has reached the next position, and so on. Though the data obtained from the probe measurements were all stored electronically, the height at which the data was obtained was recorded by hand. With the implementation of a more automated control system for the VMA, data acquisition from the probe would be entirely controlled by one person.

Parabolic Troughs: Solar Water Heaters. DIEDRE VINSON (*Eastern New Mexico University, Portales, NM 88130*) ANDY WALKER (*National Renewable Energy Laboratory, Golden, CO 89401*).

This paper focuses on concentrating solar water heating (SWH) using parabolic troughs, a renewable energy technology. Parabolic troughs only use direct solar radiation and are most effective in the Sunbelt region of the world and particularly in the southwest region of the United States. Parabolic troughs are long, curved mirrors that concentrate sunlight on a tube with a liquid inside that runs parallel in the focal line of the mirror. The liquid that is heated runs to a central tank or heat exchanger that heats potable water for large facilities such as hospitals, schools, and prisons. The particular trough system discussed is located at the Phoenix Federal Correctional Institute in Arizona. This solar water heater using parabolic trough technology preheats water for the electric water heater for this prison. From when it was installed in March 1999, to February 29, 2000, the system delivered 1,161,803 kWh (3,964 million Btu) of solar heat, saving the prison \$7,780.56 and avoiding the emission 627,374 kg/yr of CO₂, 2,324 kg/yr of SO₂, and 2,297 kg/yr of NO_x. Trough systems have proven to be a viable, cost effective use of solar technology.

Shield Design for HOMER Martian Surface Nuclear Reactor. TODD WAGNON (*Oregon State University, Corvallis, OR 97331*) ANDREW PRICHARD (*Pacific Northwest National Laboratory, Richland, WA 99352*).

We conducted research into the design and optimization of a shield for a HOMER Reactor designed to be operated on Mars with the shield being built once the reactor is operational on the Martian surface. For this we conducted MCNP calculations for doses, to limit the dose to sensitive equipment and help us optimize our shield design. We also conducted calculations to minimize the amount of shield that must be brought to the Martian surface and thus minimize costs to transport the reactor to the Martian surface. We found that the shield container can be limited to approximately 19 kg plus 250 kg of LiH shielding around the core itself. We found CO₂ and H₂O both ran into problems in that the majority of the dose is given before the shield is constructed. This leads us to believe that the design requires further optimization, most notably a faster fill rate or a more efficient pattern of filling the tank.

Analysis of Indoor Pollutant Flow Data From Social Hall Plaza. WILLIAM WATTS (City College of San Francisco, San Francisco, CA 94112) TRACY THATCHER (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Sulfur Hexafluoride and Propylene were released inside Social Hall Plaza, a six-story office building, in order to understand pollutant flow in large commercial buildings. Understanding the driving forces contributing to the flow of tracer gas in SHP will help scientists predict the flow of chemical, biological, or radioactive contaminants in a building due to a terrorist attack. Pollutants move through different flow elements in the building such as cracks under doors, elevator shafts, stairwell, and elevator shafts. Pollutants are driven through these flow elements by temperature and pressure differences. Temperature differences in the building were measured with HOBO's, and pressure differences were measured with APT's. Marin's, DPID's, and blue boxes that sampled building air measured pollutant concentrations in the building. Tracer gas concentrations in the air were measured directly by the Marin's and DPID's, but the blue boxes stored the sampled air in Tedlar bags. Mass Spectroscopy and Gas Chromatography were used to measure the tracer gas concentrations in the Tedlar sample bags. Pressure, temperature, meteorological, and tracer gas concentration data were correlated to empirically demonstrate the forces that drive pollutant flow in buildings. The real-time data collected were also used to improve predictions made by computational building models, such as COMIS.

Noise as a Function of Inversion Coefficient. BRYANT WILLIAMSON (University of Tennessee Knoxville, Knoxville, TN 37916). NANCE ERICSON (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Noise is an important parameter in the performance of electronic devices. In MOSFETs flicker and white noise are the main contributors of noise. Despite many attempts to model this noise it is unclear as to how the noise in Silicon-On-Sapphire (SOS) transistors change as a function of inversion coefficient. In this paper, a study of CMOS noise characteristics as a function of inversion coefficient from subthreshold to strong inversion, using variable gate lengths is presented. Initially, HSPICE simulation models were modified to match noise data previously collected from fabricated SOS MOSFETs under varied bias conditions. An improved noise measurement system was constructed to allow more complete noise characterization of these SOS MOSFET devices. A transistor biasing circuit and gain of 100 amplifier were built to allow various noise measurements. By connecting the device under test to the circuit and probing its output, noise measurements for a number of inversion levels and gate lengths were collected. Analysis was performed on the measured device noise and used to better predict and model SOS device noise performance. Conclusions of this work suggest better noise models than those provided by the integrated circuit foundry are needed to adequately predict device behavior. By understanding the device noise characteristics as a function of gate length and inversion coefficient, the designer can better develop circuits optimized for low-noise behavior. Noise modeling is a very important part of circuit design and making improvements in this area is one key to more highly evolved circuits.

Restoration of the Hewlett Packard Optimized Robot for Chemical Analysis system: ORCA Project. DONALD YIP (Sacramento City College, Sacramento, CA 95822) MICHAEL W. RINKER (Pacific Northwest National Laboratory, Richland, WA 99352).

Many robots in use today are for repetitive work. Hewlett Packard (HP) designed the Optimized Robot for Chemical Analysis (ORCA) to perform such tasks. The Mechanical and Robotic Systems (MARS) group at Pacific Northwest National Laboratory purchased the ORCA in the mid 1990s for use as a marketing tool for potential clients and to gain insight in robot technology for their own research. Due to lab space renovation, the ORCA was disassembled and placed in storage. In reassembling and troubleshooting the ORCA, the available manuals provided the necessary mechanical and electrical schematics. Once the ORCA is re-assembled and in operational condition, basic software routines will be written to demonstrate the ORCA's 6 degrees of freedom in movement. Because the ORCA was designed using mid-1990 technology, interfacing was incompatible between the newer computer technology, the Hewlett Packard Interface Bus (HP-IB) card, and the ORCA control unit. The HP-IB card was designed to synchronize with a Pentium1, low frequency computer, not with our existing

Pentium2, 300-megahertz computer. Technical support from HP is no longer available because the ORCA is now under the ownership of Beckman Coulter. Beckman Coulter has updated many components of the original HP ORCA. Synchronization of the hardware will be achieved by either reducing the internal clock speeds of the Pentium2 chip or by procuring a Pentium1, low frequency computer. Even after obtaining such a computer, potential problems are prone to arise due to the aged hardware and new technology.

Zero Energy Building. JAMES ZAMBO (Mississippi State Technical Community College, Knoxville, TN 37933) JAN KOSNY (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Zero Energy Building (ZEB) is the home of the future where a house produces as much or more energy than it consumes. In order to achieve this goal, the house design and its working components must be reengineered for the conservation of energy in the house. At the Building Technology Center (BTC), researchers use the Rotatable Guarded Hot Box (RGHB) and the Large Scale Climate Simulator (LSCS) for building envelope research. The RGHB tests full-size wall and window systems. The RGHB has a cold and a hot side representing the air temperatures of the building inside and outside. With the sensors applied to the assemblies, an R-value (resistance to heat flow) can be determined of the assembly. One unique feature is that the test assemblies can be rotated and thermal performance measured at any angle from 0 to 180 degrees. The LSCS tests full-size wall, roof, and floor systems. In addition, a small-scale house 12 by 12 by 8 can be tested. Likewise, the LSCS tests the assemblies for an R-value. Once a small-scale house is found to have improvements in design compared to conventional buildings the next step is to build a full-scale house and compare results. The BTC in partnership with Habitat for Humanity and TVA is building a living laboratory. Started in 1999, four houses have been built with one currently under construction incorporating different technologies. Today, Habitat has twenty lots and with new technologies from DOE and TVA a Zero Energy Building may be possible in the near future.

Pulse Width Modulation Controller. JIAN LING ZHANG (New Jersey Institute of Technology, Newark, NJ 07102) RONALD HATCHER (Princeton Plasma Physics Laboratory, Princeton, NJ 08543).

The main purpose of this study was using Power System Blockset in Matlab to simulate a Pulse Width Modulation (PWM) chopper power supply. With PWM the period between switch firings is constant while the switch closure duration is varied. Using PWM the average voltage across the load is controlled to manipulate the current. Two circuits were simulated; one without feedback, and one, which used the load current as the feedback. In simulating both cases, different parameters were set to determine their influences on the current in the load such as switching frequencies, input pulse periods, and different PWM pulses to the switches.

ENVIRONMENTAL SCIENCE

An Integrated Modeling System to Study the Impacts of Climate Variability on Water Resources in the San Joaquin Basin, California. PALLAVI RAMARAJU (Contra Costa College, San Pablo, CA 94806). NIGEL QUINN (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Water resource planners need to develop contingency plans to deal with the potential impacts of climate variability and changes in the frequency and magnitude of extreme weather events in the San Joaquin Basin. Studies suggest that warmer winter storms, earlier runoff from the Sierra snowpack, and reduced summertime flow in the tributary streams could adversely affect the water supply, water quality and agriculture production. Planning studies involving suites of complex mathematical models are often compromised owing to the inordinate amount of time devoted to data processing as the output from model is manipulated to become the input to the next in sequence. Hence the objective of this research is to develop an integrated modeling system using Object User Interface (OUI), a software package developed by the U.S. Geological Survey. OUI, a map based interface, provides an environment for efficient database/model integration, aids in map-based communication with databases, and offers controls for model execution. OUI also has tools that provide for the graphical and statistical analysis of the results. Successful linkages of various water resource management models, newly

developed within State and Federal water agencies can assist in the management of water quality, water supply and agriculture production in the San Joaquin Basin and Bay-Delta. The model system will also aid analysts in performing vulnerability analysis and suggesting management strategies for mitigating the impacts of increased climate variability and more frequent extreme weather conditions hence reducing the vulnerability of the existing system to permanent damage.

Mineralogical and Bulk-Rock Geochemical Signatures of Ringold and Hanford Formation Sediments. ROB MACKLEY (*Utah State University, Logan, UT 84341*) GEORGE LAST (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Fingerprinting Hanford and Ringold Formation sediments, two units important in terms of contaminant transport, is of timely concern for geologists hoping to characterize vadose zone sediments on the Hanford Site. A database containing many years worth of mineralogy and geochemistry data was compiled. A portion of this database was used in a multivariate study to find distinctions between Hanford and Ringold bulk-sized sediments sampled from the 200 West Area of the Hanford Site, South-Central Washington, USA. Principal component, cluster, and discriminant function analyses were performed to define minerals and major elements best at describing compositional variations within sediments. Quartz, plagioclase, mafic lithics, Si, Fe, and Ca are very diagnostic in distinguishing stratigraphic units. Using a linear discriminant function, 120 samples were classified as belonging to either the Ringold or Hanford Formation. The large majority of the samples were correctly classified, showing promise for future efforts in differentiating drill cuttings.

Assessment of Wetland Areas Along the Peconic River Proposed for Remediation. LAURIE APPEL (*Suffolk County Community College, Riverhead, NY 11901*) and GAIL RICCIOTTI (*Suffolk County Community College, Selden, NY 11784*) KEVIN SHAW (*Brookhaven National Laboratory, Upton, NY 11973*).

Brookhaven National Laboratory is supporting the Department of Energy in the remediation process of contaminated sediment found in the upper reaches of the Peconic River associated with historic laboratory activities. A detailed assessment of the wetland areas along the Peconic River was conducted to provide a pre-remediation baseline of the existing vegetation. This assessment involved: 1) identifying dominant plant communities, 2) mapping the wetland habitats, and 3) identifying the specific plant species associated with these habitats. Eighteen dominant species identified in this study comprise four distinct communities: shrub/forested, upper marsh, lower marsh, and open water. The information gathered will be used to support wetland restoration planning and design.

Particle Collection Mechanism and Preliminary Optical System Analysis of a Novel Aerosol Sampler. DANIEL ATWATER (*California State University Monterey Bay, Seaside, CA 93955*) LARA A. GUNDEL (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

A collection mechanism has been developed for a new device, the Miniaturized System for Particle Exposure Assessment (MSPEA), recently conceived at LBNL. This project is motivated by the need for low-cost technologies capable of providing accurate particle exposure data for large-scale epidemiological studies on the health effects of particulate matter (PM). This paper chronicles the first steps in realizing the MSPEA by establishing and validating the particle collection mechanism based on thermophoresis, and the temperature gradient-driven forces on airborne particles. Using a Quartz Crystal Microbalance (QCM) as a collection substrate, we measured the accumulation of mass by observing a change in frequency in the QCM. We determined that the limit of detection and quantification of the QCM system in ambient indoor air were approximately 1 and 3 nanograms, respectively. Next we implemented linear controlled thermophoresis (LCT) technique by placing a fine wire (25 mm diameter and 10 mm in length) parallel to the QCM at a distance of approximately 0.5 mm and heated the wire to 120 – 220 °C. We observed and reproduced a change in mass and a visible line of deposited particles (parallel to the heated wire). This deposition is directly related to the induction of thermophoretic forces. To characterize this phenomenon more thoroughly we have begun further experiments to optimize the system and build a working prototype air sampler by the end of year, 2002.

Rapid Mapping of Pollutant Transport and Dispersion In Large Indoor Spaces. RANDALL BARRON (*Santa Rosa Junior College, Santa Rosa, CA 95401*) TRACY L. THATCHER (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

Measuring the transport and dispersion of pollutants in a large, indoor space is of both practical and theoretical interest. The distribution of contaminants in the human breathing zone is spatially and temporally dynamic. Reliable, accurate data assists in exposure reduction. These data also contribute significantly to the verification of computational fluid dynamics (CFD) models. Previous experiments using pump and tube sampling were lengthy and invasive. New technology utilizes surface-mount optics in a large (7m x 9m x 11m) indoor space, a near-infrared (1653nm) tunable diode laser routed through two 30-channel multiplexers, and a software system capable of high-speed measurement. This allows the collection of data from 60 sensors in less than 7 seconds. A methane (CH₄) tracer gas is released through a mass flow controller from a positional source. Two-tone frequency modulation of the laser line is used to determine CH₄ absorption integrals along the path. Thirty wall-mounted remote paths are measured at the 2m, 4m and 6m plane. The geometry of the remote paths allows for determination of CH₄ concentrations at path intersections. Computed tomography (CT) is then used to reconstruct a map of the average path integrals. The generated map is then compared to data obtained from 30-point paths mounted directly above the remotes to verify the accuracy of the reconstruction. After more experimentation, these point paths can be removed to allow fully non-invasive testing. Experiments conducted thus far have demonstrated that the CT reconstructions provide a fairly accurate map of the actual gas concentrations.

The Effect of Pine Mortality on Standing Carbon Pools of Eastern Tennessee Forests. BRIDGETTE BOUDREAUX (*University of Louisiana at Lafayette, Lafayette, LA 70503*) PAUL HANSON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

During the years 1997-2000 eastern Tennessee suffered an outbreak of the southern pine beetle in a region made up of mostly hardwood forests with some interspersed pines. Such insect infestations raise the question: How does pine mortality influence the standing carbon pool of a typical eastern Tennessee forest? To evaluate this question a nondestructive method of measuring carbon content of a tree was needed, along with a forest inventory data set that predated the infestation. An allometric relationship that relates diameter at breast height (DBH) to biomass was used as the nondestructive method of carbon estimation. In 1992, thirty permanent plots surrounding an eddy covariance measurement tower on the Walker Branch Watershed were established to characterize the species mixture and density of the forest in the footprint of the tower. The 1992 permanent plot data provided a baseline from which to study the change in net carbon accumulation over 10 years and losses of carbon from pine beetle mortality. Pine mortality produced a 10% decrease in the number of trees of all species, and reduced the pine population by 93%. The loss of pine from the deciduous-dominated forest stand produced a ten percent decrease in the forest standing carbon pool, and the effect of pine mortality on the live biomass pools was nearly the same as stand net carbon accumulation from 1992 to 2002. While the southern pine beetle caused major mortality in pine forests, their effect on Eastern Tennessee deciduous forest is not catastrophic.

Anthropogenic Carbon Emissions for the United States, Canada, and Mexico. CHRISTINE BRONIAK (*The Pennsylvania State University, University Park, PA 16802*) GREGG MARLAND (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

We are attempting to determine anthropogenic carbon release for the United States, Canada, and Mexico. For the United States, we have obtained data on the amount of coal, petroleum products, and natural gas that are consumed each month. Consumption data on coal and natural gas at the monthly level was obtained from the Energy Information Administration publication Monthly Energy Review. Monthly petroleum consumption data was obtained from personal correspondence with the Energy Information Administration. We obtained corresponding state level data from the State Energy Data Report. We then obtained information on heat content, and carbon content of the various fuel types. From this information, we were able to determine the amount of carbon emitted from each fuel type. We are in the process of obtaining comparable data for Canada and Mexico. We are also interpolating yearly population data for each state in order to

determine per capita carbon emissions. This data will be used in combination with analysis of economic variables that drive carbon emissions in each state. This will allow us to gain some insights into the policy implications of these emissions and to make some recommendations for regulations pertaining to fuel use. Data at the state and monthly level will also allow greater precision in carbon modeling.

Measuring Changes in Fish Escape Behavior to Turbulence Using High Speed Cameras. JESSICA BUSEY (*Middle Tennessee State University, Murfreesboro, TN 37132*) GLENN CADA (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Indirect mortality of fish due to turbine passage may be an important consequence of hydropower production. A possible source of indirect fish mortality is extreme turbulence in the tailrace of a dam. The turbulence may cause disorientation to the turbine-passed fish, making them more susceptible to predation. In the past, predation experiments were used to test the ability of a fish to survive after being treated with a specific stress. The purpose of this experiment is to explore the usefulness of a high-speed camera in filming fish swimming behavior and compare these results to those of a classic predation experiment. The high-speed camera was set up over a fish tank designed to create turbulence in the lab. The fish were exposed to high intensity turbulence for different time periods (0, 10, 20 and 30 minutes). The responses of striped shiners and fathead minnows to a startling stimulus were videotaped. The films were then analyzed for the formation of the C shape escape behavior that is commonly used by fish to avoid predators. The fish that were exposed to turbulence were found to take longer or were unable to form the C shape. These results were compared to the results of the classic predation tests. The predation tests were much more difficult to run because predator survival and training was a problem. The high-speed camera method was found to be more reliable and easier than the traditional predation method.

Water Quality and the Effect on Fish Diversity and Population at Indian Creek. FEI-TING CHANG (*University of Illinois at Chicago, Chicago, IL 60607*) ROD WALTON (*Fermi National Accelerator Laboratory, Batavia, Illinois 60510*).

Water quality is important when examining fish diversity and population. Two components that were studied in the fish diversity and population of Indian Creek were chemical and physical environment of the water. Five study sites along Indian Creek were chosen based on the environment surrounding the creek. The chemical factor consisted of dissolved oxygen (mg/l), water temperature (degrees Celsius), using the brand model 820 dissolved oxygen meter, and pH. The physical aspect of the study involved measurement of water flow of Indian Creek. Seining was used to study the species diversity of Indian Creek. The species that were caught and accounted for in the data were crayfish, tadpoles and fish. All crayfish caught were assumed to be from the same species, as were the tadpoles. Fish on the other hand were considered as separate species once they have been identified. Data collections were usually in the mornings. The data collected show that dissolved oxygen, water temperature, species richness, and flow rate varies from station to station. Stations two and five have the highest species diversity and dissolved oxygen content. The data also indicated that correlation occurs with dissolved oxygen content to species richness, as well as flow rate to species richness. The data show that the two factors combined, contribute to species diversity in the Indian Creek.

Energized Learning: Developing Web-based Energy-Environment Education Materials for Grades 8-12. MAI CHANG (*California State University of Fresno, Fresno, CA 93710*) EVAN MILLS (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*). The purpose of the Energized Learning site is to develop web-based energy-environment education materials for grades 8-12. Since a few teachers and students have utilized the Home Energy Saver site, a web site for consumers to figure out how much energy they are using, we want to create the Energized Learning as a response to teachers and students' needs. The Energized Learning will be an ongoing site that deploys a new educational interface for teachers and students. It will be a "virtual laboratory" site, extended from the Home Energy Saver. On the Energized Learning site, there would be lesson plans on the teacher side and activities on the student side written based on the National and California standards for Mathematics and Science and the AAAS Benchmarks standard, where teachers and students can do science and math hands-on. Students will use the

"virtual laboratory" to analyze their home's energy use associated with greenhouse-gas emissions in terms of "carbon bubble." Geometry is then used to determine the diameter of the bubble, which it varies depending on the home's efficiency. Using the "virtual laboratory" associated with lesson plans, students will understand how the use of energy can have an effect on the environment. The students will also gain knowledge to make a better choice on energy use.

Aerosol-Based Duct Sealing in Large Commercial Buildings. ALAN CHENG (*Dartmouth College, Hanover, NH 03755*) DUO WANG (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Aerosol duct sealing was invented and developed at LBNL to internally seal leaky air duct systems. While the technology has been commercialized for residential and small commercial buildings, sealing ducts in large commercial buildings is often much more difficult and time consuming due to the complexity of the systems. By using highly efficient compact injectors and the multiple injection strategy, we have proved that we can successfully seal the duct system in large commercial buildings. However, one of the remaining challenges in this application is the nozzle clogging issue. Another question is whether short plenums will make some duct systems impossible to seal? The following research was done to refine the sealing process: field measurements of duct systems, nozzle clogging tests, and single-leak and multiple-branch aerosol sealing tests. The lab nozzle clogging tests show that, two nozzles (conceivably all) that are commercially available clogged up after less than 10 on and off cycles. Recently developed nozzles by LBNL researchers did not show any indication of clogging after 30 of those cycles. A lab apparatus was designed and built to simulate a plenum, where the distance from the injector and ducts branch off is adjustable. The sealing result shows that all branches of the duct system can be sealed from various distances: 36in, 26in, 17in, & 5in. In all cases, the "leaks" (perforated sheet metal plates at the end of the branches) were sealed in less than 12 minutes. However, the shorter the take-off distance the longer it took. These developments will not only improve commercial sealing performance but also has potential in residential sealing applications.

Evaluation of the Biochemical Conversion and Microbial Desulfurization of Coals. FRANK CLEMENTI (*Suffolk Community College, Riverhead, NY 11901*) MOW LIIN (*Brookhaven National Laboratory, Upton, NY 11973*).

Studies at Brookhaven National Laboratory (BNL) are conducted using a variety of bacteria chosen from various geothermal biotopes. After bacterial inoculation of pulverized coal samples, pyrolysis gas chromatography/mass spectrometry analyses are applied. This practical technique simply shows that sulfur bonds have been broken within the complex organic structure of coal. Bacterial extrapolated sulfur then reduces to a homogenous mixture of soluble sulfate and mineral medium. This biochemical conversion drastically reduces the sulfur content while improving hydrocarbon quantity and coal gasification processes. Experimental results with detailed processes will be presented along with the extensive utilization of bacteria.

Evaluation of Data Quality Reports Using the MetaData Navigator Database. VIVIAN DANG (*Columbia Basin College, Pasco, WA 99352*) ROBIN PEREZ (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Upgrades to the Atmospheric Radiation Measurement (ARM) quality databases resulted in discrepancies and inaccuracies in some information. Prior to 2000, ARM data quality information was recorded using a simple web form system. In 2000, the MetaData Navigator (MDN) was released. The MDN is a powerful java-based graphical user interface that uses databases for storing data quality information. The metadata that were entered using the older web-based tool were ported into the MDN database coarsely. Some of the detail provided in the older reports was omitted when they were incorporated into the MDN database. To improve the value of the data, quality assurance is performed on the quality assurance metadata. Data Quality Reports (DQRs) are reviewed and errors introduced in the MDN database during the porting process are corrected. Data quality information, which is complete, accurate, and clear, enhances the quality of the ARM data and, furthermore, advances the goals of ARM.

Vegetation Data Collection and Summaries for Use With LANDSAT Imagery: Providing Better Vegetation Cover Type Maps for Land Management in Southern Idaho. GINA DIDESIDERO (*Simpson College, Redding, CA 96003*) JANELLE DOWNS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Maps of existing vegetation cover are critical for fuels management, fire planning, resource monitoring, and land management. PNNL (Pacific Northwest National Laboratory) is working with the BLM (Bureau of Land Management) to develop new methods to apply to Landsat imagery that will provide more accurate classification of the vegetation cover types on public lands. New vegetation classification maps are being developed for 3 resource areas in Southern Idaho including the newly expanded Craters of the Moon National Monument. Field survey data on vegetation were collected and summarized to relate satellite spectral data to vegetation types found on the ground. The remote sensing data from Landsat is evaluated with respect to the ground truth data from these plant surveys. Correlations for the vegetation cover types and various spectral indices will be used along with environmental parameters such as soils, elevation, aspect, and image date to build an expert classification model. This model will be applied to the entire imagery set for the study area to develop a new vegetation and land use cover map.

Using Seismic Waves to Generate Background Data for Locating DNAPLs Underground. LOGAN DITTO (*Spokane Community College, Spokane, WA 99217*) ERNEST MAJER (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*). Cancer-causing chemicals have been dumped into the ground at 132 Department of Energy (DOE) laboratory sites around the United States. Methods are being used to remediate the chemicals, yet these methods remain inefficient due to an inability to accurately locate the chemicals. In an effort to find more efficient ways of locating the chemicals, the Geophysics/Geomechanics Department at the Lawrence Berkeley Laboratory is running a series of experiments that will identify whether seismic waves can effectively be used to locate and track the chemicals. The objective of this step was to simulate underground conditions and perform background measurements that will later be used in comparison with the next part of the experiment. A tank was built and filled with alternating layers of sand. Two PVC pipes were placed through all the layers to act as bore holes. The sand was then saturated with water. Using a piezoelectric bender source and 7 accelerometers, the velocity of seismic waves traveling through the sand layers was recorded and analyzed. The results are ready to be compared with data that will be collected after the injection of DNAPLs at a future date.

Sounds of Hydropower Dams and their Effects on Fish Populations. KEVIN DUDNEY (*Rice University, Houston, TX 77005*) MARK BEVELHIMER (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Hydropower provides a renewable energy source with very few pollutants, however dams can have detrimental effects on fish populations, especially migratory fish such as salmon. A better understanding of the effects of dams and power production on fish and fish behavior will provide the ability to alleviate cultural, economic, and ecological losses caused by dams on the rivers of the world. The goal of this study was to determine if sound could be used to attract fish to bypasses and to examine the sounds emitted by dams, both when turbines are on and generating electricity and when turbines are not running. We analyzed the frequencies of sounds emitted by dams using a spectrogram and compared these sounds to the range of sounds that fish can sense and to those of natural streams. Dams introduce high amplitude sounds into the water both upstream and downstream; these sounds are especially loud in the lower frequency range, which most fish experience. In a laboratory, the behavioral effects of sounds on fish, specifically sculpins, *Cottus caroliniae*, were studied by comparing the preference of fish, denoted by their movement toward areas where recordings of stream sounds were played in the artificial stream channel. Results of the laboratory study are inconclusive, but do suggest that natural stream sound is a possible attractant for fish. Also, it is clear that dams produce high magnitude sounds that very likely affect any water organisms that depend on sound. The possibility of modifying underwater sounds around dams by introducing natural stream sounds, active noise cancellation to quiet the dams, or some combination of the two warrants further investigation.

The Utilization and Evaluation of Different Techniques for the Calculation of the *Odocoileus virginianus* Population at Brookhaven National Laboratory. MEGAN DYER (*Community College of Rhode Island, Warwick, RI 02886-1807*) TIMOTHY GREEN (*Brookhaven National Laboratory, Upton, NY 11973*).

At Brookhaven National Laboratory (BNL), there have been numerous problems with the white-tailed deer population including increased car/deer accidents, foraging on ornamentals, and spread of Lyme disease. BNL decided to take surveys of the deer populations in order to get a more accurate estimate of how overpopulated the deer actually were. They divided all of the roads on-site into three transects: green, blue, and yellow. The surveys were taken from a car using a Bushnell Yardage Pro Sport distance meter, and a pair of binoculars was used to tell the number of deer per cluster and to distinguish the bucks from the does. An NK Kestrel 3000 was also used at the beginning of each survey to take weather conditions like dew point, temperature and wind speed. Using four different techniques, the data was evaluated and compared in order to get an accurate population estimate. The numbers calculated were very different and varied from 537 to 1,866 deer total, the latter being believed to be more accurate. This data will be used in the future in order to design and implement a deer management plan at Brookhaven National Laboratory.

Analysis of Soil Samples for Lead from the Chicagoland Region and Plant Uptake of Zinc with Relation to Phytoremediation for the Development of an Education Outreach Curriculum. ELIZABETH FLENS (*The Catholic University of America, Washington, DC 20064*) DEON ETTINGER (*Argonne National Laboratory, Argonne, IL 60439*).

Soil contaminated by certain heavy metals is a growing concern for commercial and master gardeners. Large concentrations of heavy metals can be toxic for plants as well as humans. The objective of this study is to develop a project at Argonne National Laboratory (ANL) in conjunction with middle and high schools to teach students about lead in soil without exposing them to lead. Zinc was used as a lead surrogate. The preliminary research was done in partnership with a research team at Northwestern University in Evanston, IL. When students submit soil and plant samples, they will be analyzed for zinc using either x-ray fluorescence or flame atomic absorption spectroscopy. Due to equipment failure, the samples in this research were analyzed using inductively coupled plasma optical emission spectrometry. In preparing the samples for analysis, the soil samples were digested using a microwave digester, and the plant samples were prepared using a beaker digestion method. The analysis showed that the highest concentration of lead among the soil samples was thirty-eight times the normal level, and all of the other urban soil samples showed a relatively high concentration of lead. Among the plant samples, geranium had the highest concentration uptake of zinc at 370.44 :g/g. Based on this initial data, marigold, mint, and probably basil and geranium are suggested for use in a classroom phytoremediation project. The development of this curriculum is ongoing, and the procedures are being adapted to make them safe for classroom use.

Fluorescence Measurements of Promoter-GFP Constructs. MARIE FORSYTHE (*Columbia Basin Community College, Pasco, WA 99301*) MARGARET ROMINE (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Bioremediation at the DOE sites has been a concern for many years. *Shewanella oneidensis*, a dissimilatory metal reducing bacteria (DMRB) is able to respire various metals and radionuclides at a remarkable rate and may potentially be an answer to this very complicated problem. A primary objective of this research is to understand at the cellular level how this bacterium reduces certain iron oxides. Approximately 52 various promoter-GFP constructs of *S. oneidensis* were tested to identify which promoters are expressed under different growth conditions. The goal of this short-term project was to evaluate the effects of growing cells in suspension versus on solid surfaces. Our results suggest that agar surfaces induce expression of four different promoters; two upstream to cell-cell signaling molecules, one to curli pilin production, and the fourth to a pair of putative c-type cytochromes. Further tests may be conducted on *Shewanella* to determine whether A12, a molecule that is secreted by *Shewanella* promotes communication between cells, effects expression of these promoters, and whether growth on agar surfaces induces promoters upstream to genes involved in biofilm formation. Results from these studies will help determine which constructs should be used for subsequent environmentally controlled studies in biofilm reactors.

An Analysis of Surface Meteorological Observations and a Regional Weather Forecast Mode. JARED FOX (*Arizona State University, Tempe, AZ 85287*) RICHARD WAGENER (*Brookhaven National Laboratory, Upton, NY 11973*).

The purpose of this project is to compare the observed Oklahoma Mesonet data with the forecasted RUC data for quality assurance purposes. Running a model to generate data is much less expensive than physically taking measurements. For this reason, it is often not feasible to collect the vast amounts of observed data that may be required for a project. Many of the ARM scientists rely upon the accuracy of the RUC model. If the model is in error, the effects could be far-reaching and may lead to incorrect results in academic and commercial projects. Due to the large size of the RUC data sets, a manageable subset was selected from a single day of data (June 28, 2002). The data was pared down by selecting only the data from the grid points that corresponded to Mesonet stations and the specific variables of interest (relative humidity, temperature, pressure, average wind speed, wind direction, and maximum wind gust speed). Analysis of the data through graphs showed that some of the RUC forecast variables were inaccurate, and that there was a correlation between certain variables that were related to each other, such as temperature and relative humidity. This showed that it is possible for errors in one variable in a model to introduce errors into other variables in that model.

Global Climate Change: Impacts of Elevated Temperatures on Respiration Rates of Tree Seedling Roots and Soil. SUSAN GEIST (*Birmingham-Southern College, Birmingham, AL 35254*) NELSON T. EDWARDS (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

As the amount of CO₂ released into the atmosphere continues to increase rapidly, global warming is becoming a growing issue of concern around the world. Tree seedlings may be more sensitive than mature trees to these rising temperatures. This is a major point of concern since the growth and maturation of tree seedlings is vital to forest succession. Soil respiration may also increase in response to rising temperatures, releasing still more CO₂ into the atmosphere. In this system, soil respiration, which tends to increase with temperature, should account for a greater part of the total respiration per unit of soil surface than growth respiration since the seedlings still have relatively few roots. Therefore, the hypothesis is that as soil temperatures increase, total CO₂ efflux from the soil surface will also increase. In order to test this, CO₂ efflux measurements were conducted on *Betula alleghaniensis* (Birch), *Liquidambar styraciflua* (Sweetgum), *Quercus rubra* (Oak), and *Populus grandidentata* (Aspen) seedlings at the Oak Ridge Open-Top Chamber (OTC) Facility. The facility consists of nine plots that expose the seedlings to three different air temperature treatments: ambient, +2.5°C, and +5°C. An Infrared Gas Analyzer (IRGA) was used to take nine weekly measurements in each of the nine plots, beginning in early June 2002. Soil temperature was measured at a depth of 5cm during each respiration measurement. Data obtained indicate a positive correlation between soil temperatures and respiration rates, as the ambient chambers have the lowest respiration rates and the +5°C chambers have the highest rates.

Assessing the Contribution of Urban Areas to Pesticide Applications Using a GIS. ALISON GOSS (*Guilford College, Greensboro, NC 27410*) BUDHENDRA BHADURI (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Pesticide contamination of surface water dominantly results from agricultural and urban applications. Agricultural applications are monitored as part of the Census of Agriculture. However, urban applications (such as those by households) are largely unaccounted for. For any watershed draining to a Community Water Source (CWS) intake, it is important to know the extent of urban areas in that watershed to assess the contribution of urban areas to total pesticide usage. Because population density can be a significant indicator of urbanization, population data for a watershed upstream from a CWS intake were derived using LandScan USA 15-arc second and 3-arc second data. In order to investigate the relationship between population and pesticide usage, a geographic information system-based algorithm was used to assign watersheds to known CWS intakes, and the population distributions for those contributing watersheds were calculated using LandScan USA data. This initial analysis represents a critical first step towards linking pesticide usage and downstream water quality data with respect to urban population. This method of

inquiry provides an avenue for assessing local, regional, and national relationships between population, pesticide use, and water quality.

Deployment and Monitoring of Phytoremediation Practices at Argonne National Laboratory. ALEXANDER HALDEMAN (*University of Illinois, Urbana, IL 61801*) M. CRISTINA NEGRI (*Argonne National Laboratory, Argonne, IL 60439*).

Groundwater quality management is essential to a healthy co-existence with our surroundings. In the 317 / 319 / French Drain area of Argonne National Laboratory, the groundwater and deep soil is contaminated with the radioactive material Tritium and various Volatile Organic Compounds (VOCs) and their degradation product trichloroacetic acid (TCAA). The goal of this project is to use trees to treat contaminated groundwater at depths of up to 10 meters. To study the results, various methods are employed: Evapotranspiration monitoring for Tritium, Soil monitoring for VOCs, Tree sap flow determination, Groundwater sampling for Tritium and VOCs, Gas Chromatograph (GC) Analyses of samples from the field, and Methanol soil extractions for identifying VOCs. Since the GC is not yet functioning properly we have no data, but we expect to find that the trees are biodegrading the contaminants in the groundwater. These results will be seen in a reduction of Tritium and VOC levels in the groundwater and soil.

Determination of Optimum Sampling Times and Temperatures for Solid Phase Microextraction and Gas Chromatography - Mass Spectroscopy of Smoked Salmon. JOSHUA HAZA (*University of Illinois at Chicago, Chicago, IL 60690*) JOHN SCHNEIDER (*Argonne National Laboratory, Argonne, IL 60439*). The Animal and Plant Health Inspection Service (APHIS) of the United States Department of Agriculture (USDA) has funded the Environmental Research team of Argonne National Laboratory to analyze the effectiveness of currently available electronic nose devices at detecting contraband meat products. The project has been divided into four tasks: characterization of volatiles, evaluation of current devices, optimization of real-world sampling, and development of a customized electronic nose. This paper focuses on the first aspect of task one: optimization of sampling times and temperatures. Samples were collected from sealed glass vials using a solid phase microextraction (SPME) device. Two replicates were performed at each of six temperatures and seven sampling times. Gas chromatography - Mass Spectroscopy was used to analyze twenty compounds, organized into four functional group classifications. Aldehydes and ketones remained relatively constant across both time and temperature parameters. Carboxylic acids peaked at high sampling times and temperatures. Alcohols demonstrated more stable peaks at lower temperatures with a slight increase with sampling time. Hydrocarbons show steady increases with increases in either sampling time or temperature.

The Uses of Microelectromechanical Systems. CHERYL HERNANDEZ (*South Mountain Community College, Phoenix, AZ 85042*) GLEN DUNHAM (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Microelectromechanical systems (more commonly called MEMS) are the incorporation of sensors and electronics among other elements on a silicon substrate made by using microfabrication technology. MEMS are used in a myriad of different areas with unique applications. MEMS have impact on biology, microelectronics, biotechnology, and aerospace technology. MEMS also help to improve the advancement of smart products. In the future, MEMS is expected to make the assimilation of microelectronics and active perceptions possible.

200 West Expansion Area Restoration Ground Cover Survey. JESSICA HERWEG (*University of Arizona, Tucson, AZ 85741*) MIKE SACKSCHEWSKY (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Plant communities in the 200 West Expansion Area were nearly eliminated after the 24 Command Fire in the summer of 2000. With the lack of vegetation to hold down the sandy soil, workers in the 200 West area were exposed to extreme blowing dust. In an effort to solve this problem, several species of grass and *Artemisia tridentata* were planted. One year after planting, monitoring of plant density showed little growth in the area. Monitoring during the second year focused on ground cover and produced more encouraging results. Four new transect lines were added to the thirteen original lines. Each transect line was approximately 50 m in length. A measuring tape was stretched between the beginning and end poles along each line and a

modified 0.2 m x 0.5 m Daubenmire frame was placed every 2 m and ground cover was calculated for each species encountered. The results showed a difference between the control and seeded areas. The control areas were comprised almost exclusively of *Salsola kali*. The seeded areas indicated growth of the planted species as well as other native species. Second year monitoring results showed that active revegetation of the 200 West Expansion Area provided greater plant cover and species diversity than the natural vegetative recovery in surrounding areas.

Capillary Barrier Profile Changes - Field Data of Soil-Forming Effects. CYNTHIA HOLST (Lewis Clark State College, Lewiston, ID 83501) LALA CHAMBERS (Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID 83415).

In 1993, the Protective Biobarrier Cap Experiment (PCBE) was established at the Experimental Field station at the Idaho National Engineering and Environmental Laboratory site. The objective of PCBE is to observe how much moisture percolates down to the protective caps, which are 0.5-2.0 meters from the soil surface. These biobarrier caps prevent leaching and evapotranspiration of hazardous waste. Roots and various organisms may break up the soil and create channels through which water can percolate down to the cap which could potentially degrade the caps, causing leakage in the forms of evapotranspiration and/or leaching. In view of potential problems, a study was undertaken to characterize the soil profile above the PCBE caps by examining the vertical stratification of phosphorus and organic carbon, then comparing these features with those of a mature soil profile from the undisturbed site having the same soil and vegetation type. Soil cores taken from the PCBE site and an undisturbed site, were analyzed for Carbon and Phosphorus. Results of this study will be reported in September 2002.

A Discussion of NREL Pilot Projects in China. SUSAN RONG XUE HUANG (McGill University, Montreal, PQ H3H 2G9) JEAN KU (National Renewable Energy Laboratory, Golden, CO 89401). In the coming years, China's energy consumption will likely rise dramatically. Renewable energy technologies can relieve the pollution that would be caused by the use of conventional fossil fuels and bring electricity to rural populations. The National Renewable Energy Laboratory (NREL) has been actively promoting renewable energy in China. NREL has participated in several pilot projects in China. The ones that will be discussed are the Inner Mongolia Autonomous Region Wind/PV Hybrid Home System project, the Gansu Solar Home System project, the XiaoQingDao Wind/Diesel Hybrid Island Power project, the Tibet PV village project and the Geothermal Heat Pump project. Topics that concern these pilot projects are financing, post-installation maintenance, project review, cultural consideration and community involvement.

Dermal Absorption of Toluene in Paint Products. MELISSA KANIA (University of Washington, Seattle, WA 98195) KARLA THRALL (Pacific Northwest National Laboratory, Richland, WA 99352).

The aim of the current research was to understand the dermal absorption of toluene from various commercial products, including enamel paint, and lacquer thinner in comparison to aqueous solutions. To understand the significance of exposure to these products, the dermal bioavailability of toluene was assessed in F344 male rats using real-time exhaled breath analysis and physiologically based pharmacokinetic (PBPK) modeling. Animals were exposed to approximately 2 ml of the toluene containing paint product using a 1.7-cm diameter occluded glass patch system attached to a clipper shaved area on the back of the rat. Immediately following the exposure, animals were individually placed in a glass off-gassing chamber and exhaled breath was monitored using an ion trap mass spectrometer (MS/MS). The concentration of toluene in the chamber was used to represent exhalation from the animal using PBPK model equations and the dermal permeability coefficient (K_p) was determined.

Tolerance Test of *Eisenia Fetida* for Sodium Chloride.

MICHELLE KERR (Jefferson Community College, Louisville, KY 40202) ARTHUR J. STEWART (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Saltwater spills that make soil excessively saline often occur at petroleum exploration and production (E&P) sites and are ecologically damaging. Brine scars appear when produced water from an E&P site

is spilled onto surrounding soil, causing loss of vegetation and subsequent soil erosion. Revegetating lands damaged by brine water can be difficult. The research reported here considers earthworms as a bioremedial treatment for increasing the salt mobility in this soil and encouraging plant growth and a healthy balance of soil nutrients. To determine the practical application of earthworms to remediate brine-contaminated soil, a 17-day test was conducted to establish salt tolerance levels for the common compost earthworm (*Eisenia fetida*) and relate those levels to soil salinity at brine spill sites. The test used 400-gram soil samples amended with sodium chloride in concentrations ranging from 1 to 15 g/kg, which represent contamination levels at some spill sites. After captive incubation at 25°C in darkness, the survival rate of the earthworms was near 90% in all tested concentrations. Also, reproduction was noted in a number of the lower-concentration test replicates and absent above the 3-g/kg concentrations. Information gathered in this project can be used as reference in further studies of the tolerance of earthworms to salty soils, as results suggest that *E. fetida* is a good candidate to enhance remediation at brine-damaged sites.

The Effects of Cation Competition on Sorption of Sr and Cs on Hanford and Ringold Formations, Hanford, WA. JENNIFER LADD (Tennessee Technological University, Cookeville, TN 38505) PHILIP JARDINE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

At the U.S. Department of Energy's Hanford Reservation in south central Washington, leaks from underground waste tanks have resulted in discharge of radionuclides to the surrounding vadose zone. Samples of two major geologic formations, the Ringold (US) and the Hanford (HF), were taken from an area near the Hanford site. Disturbed and undisturbed samples were obtained in order to quantify the coupled hydrologic and geochemical mechanisms contributing to contaminant mobility. The purpose of this study was to quantify flow and transport of coupled Cs and Sr in comparison to single-species transport. Batch and saturated packed column experiments were prepared using disturbed sediment. Maximum Cs and Sr concentration was 20ppm. Column influent solutions contained Cs⁺ and Sr²⁺ reactive tracers and nonreactive 0.5mM Br⁻ tracer. The presence of both cations resulted in significantly delayed transport of both Cs and Sr in the HF sediment. The presence of both cations did not affect the rate of transport of Sr in the US sediment, but the transport of Cs was delayed in the presence of Sr. The difference in sorption can be related to mineralogical characteristics of the media. HF contains biotite mica, while US contains muscovite mica. HF also contains more expandable clays than US. Batch adsorption isotherms did not adequately predict the trend of competitive effects. This failure suggests the importance of performing mixed contaminant flow and transport experiments to accurately predict migration of radionuclides in the subsurface.

Waste Filtration in Clastic Dikes. RASHAD LATHAN (Washington State University, Richland, WA 99352) STEVEN REIDEL (Pacific Northwest National Laboratory, Richland, WA 99352).

Abstract Clastic dikes are common structures occurring throughout the Pasco Basin. In particular, Clastic Injection Dikes occur within fissures that are produced by several mechanisms involving multigenetic processes and are filled by deposition of clastic sediments. Most of these dikes are near- vertical tabular and tapered bodies filled with multiple layers of sand, silt, clay, and minor debris and are associated with hydraulic injection. Clastic injection dikes that have formed in vadose zone sediments have the potential to influence the movement of soil moisture and contaminants. Two tests were performed to first simulate the development of a clastic dike and second to see if the rare vertical beds of sediment provide a down preferential pathway. Our conclusions showed that contaminants could seep through the vertical layers of sediment more readily, than normal horizontal beds of sediment. After looking at this information closely, the results indicate that placing waste over these types of clastic dikes is not recommended. If there is a need to store waste in the Pasco Basin area where these dikes are located, then it is recommended that they should be placed where horizontal sediment beds are located.

MTBE Co-metabolism by Pentane and Hexane Strains. DEEPAK MALHOTRA (Santa Monica College, Santa Monica, CA 90405) WILLIAM STRINGFELLOW (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Methyl tert-butyl ether (MTBE) is a gasoline additive used to promote

combustion efficiency and reduce carbon monoxide emissions from automobiles. Gasoline leaks from fuel storage tanks contaminate ground water, making it unusable for human consumption. Biological treatment is an economical way to remove MTBE from water. Previous experiments have suggested that MTBE degradation activity is mediated by bacteria able to grow on alkanes. Bacteria able to metabolize iso-pentane were also able to degrade MTBE co-metabolically. Mixed cultures enriched on hexane and longer n-alkanes showed some activity for MTBE degradation. The objective of this study was to test individual alkane degrading bacteria for their ability to metabolize MTBE and iso-pentane. Pentane degrading strains *Tsukamurella wratislaviensis* (PN 3), *Nocardia brasiliensis* (PN 7) and hexane degrading strains *Rhodococcus rhodochrous* (HX 2) and *Nocardia nova* (HX 3) were tested for growth on iso-pentane, pentane, hexane, octane, decane, dodecane, tetradecane, pentadecane, hexadecane, toluene, and MTBE. Bacterial cultures grown on pentane, hexane, or LB broth were tested for MTBE and iso-pentane degradation in microcosms. Growth on iso-pentane was observed by all four strains except PN 7. Strains HX 2 and HX 3 showed minimal growth on MTBE. Strains HX 2, HX 3, PN 3, and PN 7 show no detectable activity for MTBE or iso-pentane co-metabolism in the microcosm test. The results of this work show that pentane and hexane degrading bacteria have a limited potential to metabolize MTBE.

Life-Cycle Cost Analysis. RAQUEL MAYO (*Fresno State University, Fresno, Ca 93650*) ANDREA DENVER (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Standards for appliances are a vital policy tool for attaining cost-effective energy savings. Prior to standards appliances were less efficient wasting millions of dollars. Studies of the financial impact of imposing new minimum standards show the energy and cost savings on society today and the future. Life Cycle Cost Analysis is used to evaluate the total cost of newly designed distribution transformers as the Monte Carlo simulation calculates a statistical distribution of results. New designs and standard levels are analyzed to find the most cost efficient standard. Preliminary results show any efficiency improvements are cost effective and feasible. We have found that by using statistical distributions in the calculation, there are significant improvements on the results of the accuracy and the consequent economic impact. The final report to the Department of Energy will aid in identifying which efficiency standard would best meet the needs of the country in order to make the most effective decision of which new minimum standard should be met.

Measurement of Air Quality During Driver Training on The Stryker Vehicle. JUAN MELENDREZ (*Yakima Valley Community College, Yakima, WA 98902*) RANDY R. KIRKHAM (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The amount of particulate matter generated during training with the new Stryker military vehicle could raise concerns if the PM10 concentration exceeded the EPA's standard. As the new vehicles drove the obstacle course at the Yakima Training Center, minivol air samplers were set up around the course in eight different locations. The results of the data showed that of all the locations only one of the eight sites had a PM10 concentration that was just above the EPA's standard. The Stryker course is located 5 kilometers east of Cantonment and generally down wind. This caused the particulate matter to blow into the Yakima Training Center where it had little or no effect on the Yakima PM non-attainment area.

NMR Applied to Porous Media. MEGHAN MILLER (*University of Florida, Gainesville, FL 32611*) LIVIU TOMUTSA (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The simulation of oil reservoirs is essential for the optimization of oil production. The LBNL research group is constructing computer models to simulate the flow of oil, water, and gas through virtual porous media. These models require an input of characteristic grain size distributions. NMR has the potential to determine accurate distributions of grain sizes. NMR measures the behavior of nuclei spins under the application of magnetic fields. After the removal of an applied magnetic field, protons return over time to equilibrium. This is referred to as the relaxation time. This project investigates whether there is a correlation between T2 data and the grain diameter. Grains in this experiment were approximated as round glass beads. Sieving the beads provided a narrow range of glass bead size. The distribution of the grain sizes was validated using a microscope. The NMR analysis was then performed for each bead distribution. A general correlation was found

to exist between the mean grain size and the NMR predicted grain size according to T2 values.

Comparison of Aerobic and Anaerobic Microbial Activities in Landfill Bioreactors. STACY MIRANDA (*Merced Community College, Merced, CA 95348*) TERRY C HAZEN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Municipal Solid Waste landfills are becoming an ever-growing problem because they produce noxious odors, greenhouse gasses and toxins that contaminate the environment. To control contamination, the EPA requires that landfills be lined and capped with an impermeable liner that slows the rate of degradation. To accelerate degradation, some landfills now operate as anaerobic bioreactors, utilizing a leachate collection/recirculation system to optimize degradation and methane production rates. Compared to anaerobic systems currently in use, aerobic systems would be more efficient because they would be able to support anaerobic microenvironments, leading to a more diverse microbial population, fewer greenhouse gas emissions and cleaner leachate. Using enzymatic activity analysis and cell enumeration techniques, it was found that enzymatic activity fluctuated over time with only dehydrogenase activity showing a steady trend, and bacterial viability counts showing higher cell viability in the aerobic tanks. Since we know from measurements of carbon dioxide production and waste mass reduction rates that the rates of biodegradation are as much as 40 times greater under aerobic conditions, we clearly have not yet found enzymes that reflect the gross metabolic activity that must be occurring. These studies demonstrate that biomass differences between the anaerobic and aerobic conditions do not account for the differences in leachate quality and biodegradation rates, thus the specific activity per cell must be much higher for the aerobic systems. This information could lead to promising new techniques to manage our landfill problem in a more efficient and cost effective way.

Vegetation Characteristics of a Constructed Wetland at Argonne National Laboratory - East, Illinois. JAMI MURRAY (*University of Illinois at Chicago, Chicago, IL 60612*) KIRK LAGORY (*Argonne National Laboratory, Argonne, IL 60439*).

Construction of the Advanced Photon Source (APS) at Argonne National Laboratory resulted in the destruction or alteration of three wetlands in the project area. To compensate for these impacts, a new wetland (Wetland R) was constructed adjacent to the APS in 1990. Plant colonization and establishment was monitored for the first five years after initial construction. The present study was conducted during the summer of 2002 to determine current conditions of the wetland, identify changes that have occurred since 1996, and determine whether additional maintenance efforts are appropriate. A randomized plant sampling method was implemented using transects and quadrats to determine the percent cover of plant species. Occurrence and percent cover for dominant species were compared to similar data from previous monitoring studies. Rice cutgrass (*Leersia oryzoides*), crown vetch (*Coronilla varia*), and narrow-leaved cattail (*Typha angustifolia*) were the most dominant species in Wetland R in 2002 and have been found there since initial monitoring in 1992. Crown vetch and rice cutgrass have increased over time. Narrow-leaved cattail has decreased and river bulrush (*Scirpus fluviatilis*) has been virtually eradicated since 1996. To improve the quality and function of Wetland R, invasive and non-native species should be eliminated or reduced through herbiciding and burning. Rare and high quality wetland species, like grass-leaved arrowhead (*Sagittaria graminea*), should be monitored to protect and preserve their populations. In addition to controlling unwanted vegetation in wetland and surrounding upland, planting and managing of native species should continue.

Development of Standard Culturing Procedures For *Chironomus tentans* (Order Diptera: Chironomidae) used in Columbia River Toxicology Studies. MICHAEL MUSIALOWSKI (*Prescott College, Prescott, AZ 86301*) AMORET BUNN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Chironomus tentans (Order Diptera: Chironomidae) is an aquatic macroinvertebrate widely used in sediment toxicology. However, standard culturing and testing procedures are different than conditions in the Columbia River. A future study of 90Sr uptake by chironomids in the Columbia River depends upon culturing larvae on a substrate whose own uptake of 90Sr can be easily factored out. Chironomids were cultured using three substrates: shredded toilet paper, local

sediment, and local periphyton. The 5cm and 0.3 cm thick sand cultures most consistently facilitated larval growth with a minimum of complications from other organisms. One of three 5cm thick toilet paper cultures developed anaerobic conditions and both 0.5 cm thick toilet paper cultures developed fungal blooms. Metamorphic sequence determination was approximated. Chironomid life history was documented in enough detail to facilitate ease of culture by other researchers. Variable culture performance indicated that variables such as larva size, discoloration, and egg-stocking density need to be more systematically studied to better understand causes and effects. Consistent water temperature is an essential prerequisite to such studies. Feeding rates were standardized and found to be specific to substrate type and thickness. Most culture observations were consistent with those found in the literature.

Solid-Phase Characterization and Carbon Sequestration in Ultisols and Inceptisols on the Oak Ridge Reservation. ROSS NESBIT (*University of South Carolina, Columbia, SC 29225*) PHILLIP JARDINE (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The enhancement of soil carbon sequestration is an appealing way of offsetting the potentially harmful effects of the anthropogenic rise in atmospheric CO₂. The thick soil profiles of deep clay and Fe-oxide-rich subsoils of humid and tropical climates have a great capacity to stabilize and accumulate organic C, decreasing the rate of carbon turnover by orders of magnitude relative to surface soils. The objectives of this project were to: (1) quantify the magnitude of enhanced carbon accumulation within deep subsoils of forested Ultisols and Inceptisols and (2) quantify those mechanisms responsible for the capture and accumulation by the solid phase. A shake-batch method was utilized to construct dissolved organic carbon (DOC) adsorption isotherms on numerous Ultisol and Inceptisol subsoils from the Oak Ridge Reservation. In an effort to cross-correlate soil properties with differences in DOC solid-phase adsorption, select physical and chemical properties of the soil samples were determined. Experimental results indicated that carbon adsorption increased with depth for a given soil type, where B-horizons had greater adsorption capacity than the upper A/B and E/B horizons. Mass accumulations of nearly 0.2% weight-by-weight were possible in B-horizon soils, which amounts to an increase in solid-phase loading 2-20 times above indigenous levels. The Fe-oxide content and the soil pH appeared to control DOC sorption, where B-horizons characteristically had higher Fe-oxide levels and lower pH values than upper soil horizons. The experimental data from this research will provide new quantitative information on the significance of carbon credits in deep soil profiles.

Finding Relationships Between Ambient Ozone Concentration Levels of Organic and NO_x Emissions Using a Trajectory Box Model, OZIPR. VANESSA NGUYEN (*University of California at Los Angeles, Los Angeles, CA 90024*) YIN-NAN LEE (*Brookhaven National Laboratory, Upton, NY 11973*).

Mathematical, computer models are necessary to predict the effects of anthropogenic and biogenic emissions on the compositions of the atmosphere. These models help develop control strategies for reducing photochemical air pollution because they can estimate changes in air quality resulting from changes in emissions. One trajectory-type, air quality simulation model, Ozone Isopleth Plotting Program, Research Version (OZIPR), is tested to show how well this program can estimate the emissions of pollutants, especially the most universal problem ozone. The case studies are run in cities in which field tests have already been performed by the Atmospheric Sciences Division of Brookhaven National Laboratory. The initial conditions and input parameters for these simulations are then based on the conditions at these sites, and the output generated by OZIPR are compared qualitatively to the concentrations of emitted species obtained from the field tests to determine the accuracy of the program. At each city, one specific variable is changed to further examine the sensitivity of the OZIPR calculations. The OZIPR predictions of the five case studies turned out to be comparable to actual results. The expected changes in ozone and other air pollutants were approximated well, proving its value as an air quality model.

Parameterization and Implementation of the Introductory Carbon Balance Model-to-Model Carbon Sequestration in Soils of Old Growth Forests in Western Pennsylvania. GABE OLCHIN (*Colorado State University, Fort Collins, CO 80523*) KIM MAGRINI (*National Renewable Energy Laboratory, Golden, CO 89401*).

Increasing atmospheric carbon dioxide levels have sparked global interest in carbon dioxide sequestration. Carbon sequestration in the earth's soils has been shown to be a large and accessible sink for reducing atmospheric carbon dioxide levels. Determining carbon content already present in soils is as essential to understanding the process of carbon sequestration as modeling how much carbon can be stored in soil in the near future. Soil carbon data from the Tionesta Scenic and Natural Areas of northwestern Pennsylvania was available for four forests ranging from 15 years to 600 years old. Each site was sampled at three depth increments and analyzed with pyrolysis Molecular Beam Mass Spectrometry (py-MBMS), which rapidly characterizes soil carbon content and chemical species. We evaluated many ecological modeling programs for predicting soil carbon dynamics and uptake with time and chose the Introductory Carbon Balance Model (ICBM). Data sets from the four sites comprised of total carbon and amounts of young, intermediate, and old carbon were integrated into the ICBM program to validate its use in modeling forest soil carbon sequestration potential. Preliminary work showed that with more samples and forest soil data, ICBM can and should be used to model forest soil carbon dynamics over a 30-year time frame. Applying this model to our quantitative soil carbon data can further validate its use as a tool to answer questions about sequestering CO₂ in the earth's soils. This sequestration can be a substantial and natural way to reduce global CO₂ levels.

Analyzing the Water Quality Environment for Migrating Salmon in the Lower Snake River. DANIEL OLIVARES (*Walla Walla Community College, Walla Walla, WA 99362*) CHRISTOPHER B. COOK (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Water is released annually from Dworshak Reservoir to decrease water temperatures in Lower Granite Reservoir (LGR) during periods when anadromous Chinook salmon are migrating. The purpose of this research was to provide water temperature data in LGR, especially in the mixing zone downstream of the Snake/Clearwater River confluence, a biologically important location. Temperature data was collected using self-contained temperature loggers positioned along a vertical cable placed at various areas of interest. The Clearwater River was found to be 4 to 10 °C cooler than the Snake River between July and August 2002. Stratified conditions began where the two rivers met and was observed to continue downstream to Lower Granite Dam. Furthermore, stratification was found upstream of the confluence, along the Snake River for over 1 km. Three-dimensional temperature variations at and around the Snake/Clearwater River confluence were mapped out during the project, and these results will be of use to various river managers (e.g., fisheries, hydropower, etc.) as they continue to examine locations of concern throughout the Lower Snake River system.

Molecular Analysis of the Microbial Community Structure in Aerobic and Anaerobic Landfill Bioreactors. ELIZABETH PADILLA (*University of Puerto Rico, Mayaguez Campus, Mayaguez, PR 00680*) CARLOS RIOS-VELAZQUEZ AND TERRY HAZEN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Landfill management is becoming one of society's greatest problems. Bioremediation approaches represent a solution to treat these sites. However, in order to design successful restoration approaches, a better understanding of the microbial communities involved in detoxification and stabilization is needed. In this study we analyzed the microbial community structure of different landfill bioreactors using 16S rDNA-based molecular techniques. Genomic DNA from the bacterial communities of leachate and gravel samples was extracted, and 16S rDNA was amplified by Polymerase Chain Reaction (PCR) using bacterial primers. Terminal restriction fragment polymorphism (T-RFLP) was used to analyze the community structure of the bioreactors along with clone libraries. In addition, the presence of TCE and PCE dechlorinating bacteria (e.g., *Dehalococcoides* sp.) was tested using specific primers. The T-RFLP results demonstrated diverse communities in all bioreactors, with the highest diversity observed in the anaerobic bioreactors. A more complex bacterial community was associated with the leachate samples than with the gravel samples. Clone libraries from the anaerobic bioreactors were generated and T-RFLP identified two dominant populations. Sequence analysis suggested that they belong to two different phylogenetic groups of non-yet cultured bacteria. An amplification product using *Dehalococcoides* specific

primers was obtained from samples of the Yolo County Landfill. This finding is significant because it indicates that landfills can support bacteria capable of the complete mineralization of chlorinated solvents and other toxic compounds.

Quantification of Algal and Bacterial Biomass. OLIVER PARADIS (Laney College, Oakland, CA 94607). WILLIAM STRINGFELLOW (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The San Joaquin River (SJR) project is an ongoing project characterizing water quality of various tributaries of the SJR. For this project, water samples are collected for organic carbon and inorganic nutrient analysis. Organic carbon is measured as total organic carbon (TOC) using an Apollo 9000 TOC Analyzer. It works by burning a sample at 680°C and the combustion product (CO₂) is measured with an infrared detector. The resulting data can be compared against a standard curve of known carbon concentrations. Most organic carbon in the SJR is particulate carbon of biological origin and is important to levels of dissolved oxygen downstream, as bacterial respiration of the carbon uses oxygen. A low level of dissolved oxygen is an indication of poor water quality and is detrimental to sensitive fish populations. Low dissolved oxygen conditions in the SJR have placed the river on the federal 303d List of Endangered Waterways. The objective of this work was to establish if the current method for measuring TOC was effective at measuring particulate organic carbon, especially carbon in the form of bacteria and algae. It was hypothesized that homogenizing algal or bacterial samples before processing them in an Apollo 9000 would improve the yield of measured carbon. It was found that homogenization does not increase the measurement of particulate organic carbon. However, dissolved organic carbon concentrations did increase, suggesting homogenization did disrupt or break some particulate carbon. These results demonstrate that the standard protocol currently being used for TOC analysis is effectively measuring of particulate organic carbon in these samples.

Sensitivity Analysis of the Lagrangian Particle Dispersion Model - Backwards (LPDM-B) to Input Parameters. KAREN PARKER (University of California - Berkeley, Berkeley, CA 94720). MARC FISCHER (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

To better understand the terrestrial carbon cycle and its effects on the global climate, measurements of CO₂ fluxes and concentrations must be made. Measurements can only be made at a finite number of points, thus, a model is needed to interpret the measurements and describe CO₂ fluxes and concentrations over a continuous region. Existing models are available that describe the region measured by a sensor fixed on a small (approx. 5m high) tower. Data is being collected by the DOE Atmospheric Radiation Measurement Program Southern Great Plains Site Central Facility on a 60m tower and a new, time-reversed Lagrangian stochastic dispersion model (LPDM-B) is analyzed to be used with data from the ARM tower. The output of the model is called the 'footprint' of a measurement. A sensitivity analysis of the model showed that the footprint is sensitive to different types of surfaces (crop type and local topography), but not very sensitive to different heights of the planetary boundary layer. Input parameters for the model were taken from the data collected at the ARM tower, and as a preliminary investigation of LPDM-B using actual data, we ran the model with data from 07/13/01. The footprint was very variable during the day and stable at night. This may mean that during the day, for a given CO₂ measurement, it may be difficult to predict where the CO₂ came from, but at night the model may give more reliable information. More analysis is needed.

Using Computed Microtomography with Fluid Flow. BRIAN PHILLIPS (Jamestown Community College, Jamestown, NY 14701). KEITH JONES (Brookhaven National Laboratory, Upton, NY 11973).

The X27A beam line at the National Synchrotron Light Source has studied many geologic samples. The new task is to look at samples from Hanford, Washington. Hanford is a nuclear waste storage facility that leaked contaminants into the soil. To aid in the efforts to find where the contaminants are, the soil samples are x-rayed by X27A. The data are manipulated to get 2D and 3D images. The images are used to study the porosity of the soil. Looking at the porosity will aid in determining how fluid flows through the soil. Many sets of data will be taken from different samples, and many techniques will be used to study the soil. The hope is to fully understand the technique used to visualize the data and be able to reproduce the results with other images.

Biological Processes Potentially Affecting the Compacted Soil Barriers at the CFA Landfills. COURTNEY PICKUP (Utah State University, Logan, UT 84321) SHERRI STACEY (Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID 83415). Waste Area Group 4, which is part of the Environmental Restoration Department at the Idaho National Engineering and Environmental Laboratory, sponsored a Science Action Team to study and survey vegetation, small mammals, rooting depths, and small mammal's burrows. These studies were conducted at the following four sites: Central Facilities Area Landfills I, II, III, and a control area East of Landfill III. The impact of deep rooting plant species and small mammal burrows (which could provide a pathway for water to leach through the compacted soil barrier into the buried waste at three of these sites) is a concern. This is because precipitation could aid in the movement of contamination down through the soil column into the Snake River Plain Aquifer lying beneath the sites. Impact on these locations from biological processes is a long-term issue that will require continued monitoring and analysis before a conclusion can be reached.

Long-Term Predictions of Global Climate using the Ocean Conveyor. PATRICK RAY (Indiana University of Pennsylvania, Indiana, PA 15705) JAMES R. WILSON (Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID 83415).

Many have attributed the Great Ocean Conveyor as a major driver of global climate change over millennia as well as a possible explanation for shorter (multidecadal) oscillations. The conveyor is thought to have a cycle time on the order of 1000 years, however recent research has suggested that it is much faster than previously believed (about 100 years). A faster conveyor leads to the possibility of the conveyor's role in even shorter oscillations such as the El Nino/Southern Oscillation (ENSO) and the North Atlantic Oscillation (NAO). The conveyor is primarily density driven and the salty outflow of the Red Sea is used to predict its behavior ten years into the future. A successful model could lead to a long-term prediction (ten years) of El Ninos, Atlantic hurricane season intensity, as well as global temperature and precipitation patterns.

Electronic Transport in Pd-PdH Film with H₂ at RT. BENJAMIN REED (Olive Harvey Community College, Chicago, IL) JONG HEE PARK (Argonne National Laboratory, Argonne, IL 60439).

When H₂ is incorporated in Pd, H₂ is (ad/ab) into pure Pd making PdH at equilibrium. H₂ is trapped at the surface of the host metal by electrons in metal Pd. Eventually, H₂ is adsorbed into the bulk of Pd. H₂ incorporation in Pd brings about a change in resistivity of Pd metal. This concept will be used to develop a sensor that will selectively detect gaseous hydrogen at RT.

Patterns of Oak Recruitment in Selected BNL Woodland Communities. JAHAIIRA RIVERA (Interamerican University, Rio Piedras, PR 00916) and BURGOS YULESKA (University of Puerto Rico, Cayey, PR 00736) JOHN BLACK and PETER KELLY (Brookhaven National Laboratory, Upton, NY 11973).

The normal progression of forest development in the Long Island Pine Barrens of central Suffolk County begins with pitch pine. Over time, the pitch pines are out-competed and replaced by a hardwood forest composed of oak and hickory. However, a preliminary survey of woodlands at Brookhaven National Laboratory showed a virtual absence of hardwood seedlings and saplings. This survey was accomplished by establishing seven circular plots with a radius of 10 meters each to determine the effects of the shrub layer on oak recruitment. Two of the plots had a recent fire history. These plots had a greater number of oak seedlings and saplings than in the areas with no fire history. Prescribed burning is often used as a technique to manage for the perpetuation of pine barren communities. Our data, however, suggest that fire may accelerate, not retard, succession toward oak dominance. In conclusion, the shrub layer in an unburned woodland may prevent oak recruitment while fire reduces the shrub layer, thereby encouraging the establishment of oaks.

Seeing Hanford Site Soil with Computed Microtomography. KAREN RUSIN (Alfred State College, Alfred, NY 14802) KEITH W. JONES (Brookhaven National Laboratory, Upton, NY 11973).

Computed microtomography is a tool that allows non-intrusive, nondestructive viewing of the interior of opaque objects on the scale of microns. Computed microtomography was used to create digital three-dimensional images of soil samples from Hanford, Washington. It

is hoped that this will lead to a better understanding of how fluids, such as the toxic wastes and heavy metals leaking from the holding tanks, interact with the soil of the Hanford site. Soil samples were held in containers while light from the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory was passed through them as they rotated through 180 degrees. The remaining light was passed through a scintillator and into a CCD (charge-coupled device) camera, which took digital snapshots and saved them to the hard drive of the computer that ran this process. A three dimensional image was created from this data after manipulation by many different software programs. These three dimensional images and the data they are based upon may be used by geologists and environmental scientists to derive better ways to predict the travel of toxic waste through the ground, and to aid in planning the recovery and removal of this waste from the Hanford Site.

Simulating Signals from Chem-Bio Sensors in a Building. MAHSA SADRE-BAZZAZ (Los Angeles Valley College, Valley Glen, CA 91401) ASHOK J. GADGIL (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

Baysian Monte Carlo Updating (BMC) is a method based on the Baysian statistics, which has been developed to estimate characteristics of a point-pulse release by interpreting sensor data. BMC application to buildings is currently based on COMIS model that treats a building as a collection of well-mixed zones. Although the assumption of uniform distribution of pollutant within individual rooms is common to simplify the problem of pollutant dispersion in buildings, it does not fully represent a realistic solution (real rooms are not instantaneously mixed), particularly for the early phases of a pollutant release. We generate synthetic signals in a five-room hypothetical apartment applying Computational Fluid Dynamic (CFD) simulations (CFD does not rely on the instantaneously well-mixed assumption). The generated signals will be employed to challenge BMC algorithm in the early phases of a pollutant release when the building zones are not well-mixed.

Determine Feasibility to Replace Hydraulic Hoses, Install Steel-Braided Coils and Replace Hydraulic Oil with Vegetable-Based Oil to Reduce Environmental Spills and Write a Pollution Prevention Proposal. REGINALD SAINT-JUSTE (Hudson County College, Jersey City, NJ 07305) PATRICIA WILLIAMS (Brookhaven National Laboratory, Upton, NY 11973).

ABSTRACT Plant Engineering has had numerous environmental spills as a result of failed hydraulic hose lines in the past several years. Even though the equipment undergoes preventative maintenance on prescribed intervals, a lot has to be done to improve, to reduce or eliminate the potential for a spill involving hydraulic pressurized lines. Plant Engineering (EP) is a division that works to provide premier facilities and services to the research community here at Brookhaven National Laboratory. They are one big team that takes care to incorporate environmental issues in their routine work like building construction, cutting grass, maintenance, and even custodial services. They also make sure that their tasks are properly done to the advantage of the entire lab. One of Brookhaven National Laboratory's programs is the Pollution Prevention program. This is why they brought me here this summer to investigate alternative lubricants and hydraulic steel-braided hose replacement for heavy equipment used by Plant Engineering. I interfaced with the various equipment manufacturers, reviewed technical specifications for the various pieces of equipment, identified environmental-friendly replacement oils and replacement hose sizes and documented the results. The main purpose of the project was to utilize the benefits of Brookhaven National Lab's Prevention Pollution Program implemented couple of years ago. If the Laboratory will get environmental benefits, the project will get funded. My job was to present the data on a Pollution Prevention Proposal form that showed the costs and benefits of using alternative lubricants and replacement hose fittings for heavy equipment.

Aerobic vs. Anaerobic Landfill Microbial Community Structure and Biomass using Phospholipid Fatty Acid Analysis. FELIX SANTIAGO (University of Puerto Rico Mayaguez Campus, Mayaguez, PR 00681) TERRY C. HAZEN (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

Landfill research, until very recently, has focused in the understanding of biodegradation under anoxic conditions, but information regarding aerobic biodegradation is scarce. This research aims to obtain a

general overview of the microbial communities present in landfill-simulating bioreactors under different environmental (oxic and anoxic) conditions, and from an active municipal solid waste landfill in Yolo County, CA. Phospholipids Fatty Acids (PLFA), which are useful in complex sample analysis and viable biomass estimation, were extracted from leachate and gravel samples by silicic acid column chromatography. Fatty Acid Methyl Esters (FAME) were obtained after chemical modification of the PLFA's. Gas Chromatography analysis of the FAME's yielded similar microbial community composition, but different relative abundance of the communities, for all leachate and gravel samples. Signature lipids for Actinomycetes and sulfate reducers were predominant in gravel samples from the anaerobic tank, due to the higher concentration of sulfides in their environment. Aerobic bioreactors presented higher abundance (approximately 20% of the total population) of fungi and microeukaryotes that aid in the biodegradation process, but these populations comprise only 5% or less on the anaerobic bioreactor. More than 80% of the total lipids extracted where from bacterial origin. To have a better overview of the microbial community structure more signature lipids, like those for Archea, need to be taken into account and predominant communities must be examined closely. Other methods for estimating viable biomass must be used to provide a more precise measurement.

Changes in Characteristics of United States Snowfall Over the Last Half of the 20th Century. DARIA SCOTT (St. Cloud State University, St. Cloud, MN 56301) DALE KAISER (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Several recent studies have reported that large portions of the mid- and high-latitude land areas of the northern hemisphere (including much of the United States) have experienced increasing precipitation over the last half of the 20th century. From a relatively small number of studies of snowfall trends, the characteristics of northern hemisphere wintertime precipitation over this period have been found to vary over space and time. Over the United States, some specific findings from these studies include: increasing snowfall in parts of the Great Plains and Northeastern states; increasing inter-annual variability in nationally averaged snowfall; and, as recently reported by the IPCC, a reduction in a directly related variable - spring snow cover area - in the latter half of the 20th century. In our current study, daily snowfall amounts from 1948 through 2001 from several hundred stations in the United States Historical Climatology Network (lying north of 35 degrees north latitude) are examined in several ways. We analyze records over the whole year and also over an October through May "snow season" to study trends and variations in variables such as total snowfall, number of snow days, average magnitude of snowfall events, number of events exceeding specific thresholds, near-surface air temperature on snowdays, and the contribution of snowfall liquid water equivalent to total annual precipitation. Preliminary results indicate interesting regional changes in many of these variables.

Accuracy and Repeatability of a New Method for Measuring Residential Air Duct Leakage: DeltaQ. PRABU SEGARAN (Pacific University, Forest Grove, OR 97116) DARRYL DICKERHOFF (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

Existing residential duct systems are only 50-75% efficient. This translates into a huge loss of energy and money: 1 GW during peak power usage and \$400 million/year in California alone. The current measurement method (duct pressurization) only measures the size of leaks; actual leakage flows at operating conditions are needed to evaluate system efficiency. DeltaQ reports separate supply and return duct leakage to outside, as well as envelope leakage. The development of automated software should make the DeltaQ method faster. Previous tests for accuracy with DeltaQ had tendencies to overestimate leakage values that were thought to be attributable to installed asymmetric leaks. Symmetric leaks were built using 6-inch and 8-inch PVC stuffed with drinking straws with length-to-diameter ratio of about 25:1. These leaks were calibrated to simulate the pressure exponent of about .66 common to most residential ducts. A varying damper in the heating system proved to greatly affect the results of this method (indicated by large negative flow values), suggesting an inspection of the system before testing. Tests (after fixing damper) showed that DeltaQ still tends to overestimate, possibly due to erroneous assumptions in the model. These results will be reviewed by the standards committee of ASTM for the Delta Q procedure to become the "Standard Test Method for Determining External Air Leakage of Air Distribution

Systems by Fan Pressurization-E1554." This would also lead to use by utilities for duct efficiency credits in energy efficient home rebate plans and by the California Energy Code, Title 24.

Creating a User-Friendly Input Format using XML: Application to the Computer Program COMIS. RUZAN SHAHINI (Santa Monica College, Santa Monica, CA 90405) PHILLIP N. PRICE (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). The computer program COMIS calculates airflow and pollutant transport in buildings using the multizone infiltration model. The multizone model considers a building as a collection of well-mixed zones that are interconnected by airflow components. It assumes that each zone is instantaneously well-mixed, meaning any biological or chemical substance in the zone is uniformly distributed through it. The COMIS Input File (CIF) provides the program with the necessary information about a building and its environment, as well as possible pollutants. In order to make the input file user-friendlier, the decision was made to change its format to Extensible Markup Language (XML). Also a program with a Graphical User Interface (GUI) is being written, that will help the user to visualize the building through a graphical display and will offer an interface for entering information and creating an XML input file based on it. Because changing COMIS to read XML input will require a few years, I wrote a computer program that converts from XML to CIF. This conversion program was written using Extensible Stylesheet Language Transformations (XSLT), which was designed for extracting data from an XML document. To be able to still use the many existing CIFs once COMIS is changed, I wrote a second program in Perl to convert from CIF to XML. Additionally I wrote an XML-Schema that specifies the structure and possible content of the XML input file. The Schema is used to verify the correctness of an XML document, by validating the document against the Schema.

Comparison of NO₂ Photolysis Rates Modeled by the FASTJ Code and Measured by a Filter Radiometer for Five Clear Days. KATHERINE SHAVER (Lyon College, Batesville, AR 72501). W. RICHARD BARCHET (Pacific Northwest National Laboratory, Richland, WA 99352).

Although ozone is a major component of air pollution, it remains extremely difficult to regulate and to predict because many parameters have a role in its formation in the troposphere. Studies have shown that the uncertainties of ozone prediction are strongly correlated with the uncertainties of NO₂ photolysis rates. The FASTJ code simplifies photolysis modeling by parameterizing the effects of clouds by assuming a uniform sky cover. In this study, the FASTJ code used aerosol optical thickness data from shadow band radiometers to model photolysis rate coefficients for NO₂ (J(NO₂)). Five clear days were chosen for analysis, and the FASTJ models for these days were compared to the reported J(NO₂) from a filter radiometer in the same area as the shadow band radiometers. The J(NO₂) values from the FASTJ code were compared to values from the filter radiometer throughout each day. Although the FASTJ code underestimated the J(NO₂) in the early morning and late evening and overestimated the J(NO₂) during midday, the FASTJ code was within 0.16% of the radiometer when integrated over the entire day. Because this study focused solely on clear days, further investigation needs to be done on overcast days using the FASTJ code's overcast sky parameter.

The Fate of Metal-EDTA Complexes During Uptake by Tagetes. DAVID SINGER (Stanford University, Stanford, CA 94305) MARK FUHRMANN (Brookhaven National Laboratory, Upton, NY 11973). Phytoremediation is the use of plants to remove toxins from soils. The addition of synthetic chelates, specifically Ethylenediaminetetraacetic acid (EDTA) increases uptake of some metals. Little is known about the mechanism by which plants take up metal-EDTA complexes. In this study FT-IR spectroscopy was used to determine if metal-EDTA complexes are transported up plants as a complex, or broken apart. Each metal-EDTA complex has its own identifiable IR scan that can be fingerprinted in plants, and also the concentrations of these complexes can be determined. Tagetes was exposed to solutions of 100 mM Fe(II)-EDTA and Zn-EDTA, and 80 mM Pb-EDTA. The concentrations of metal-EDTA in the plant shoot liquid were determined to be 67mM, 82mM and 44mM for Fe(II), Zn and Pb respectively. By ICP, the metal concentrations were determined to be 91.17mM, 82.59mM and 35.08mM for Fe, Zn and Pb, respectively. Further, the concentrations of the metal-EDTA plant-exposed solutions were determined by ICP and were found to be the same both before and after uptake. These data, in conjunction with the shoot liquid data shows that the metal-EDTA

complexes were transported from the solution through the roots and up into the plant as a complex, and not dissociated. We were not able to use FT-IR to observed metal-EDTA in the solid part of the plants, so it is unclear if the metal-EDTA complexes remain complexed there. Future work requires synchrotron based FT-IR spectroscopy to observe metal-EDTA complexes with the solid part of the plants, and also in small concentrations. However, we have clearly shown that metal-EDTA complexes are transported in plants as a complex, and not broken.

Comparison of X-ray Computed Microtomography, Confocal Microscopy, and Light Microscopy on Insects Encased in Amber. MARC SPENCER (State University of New York - Binghamton, Binghamton, NY 13902) KEITH W. JONES (Brookhaven National Laboratory, Upton, NY 11973).

Through the use of computed microtomography, confocal microscopy, and light microscopy, insects that have become encased in amber can be studied without destroying the specimen. Light microscopy, although esthetically pleasing, cannot provide such detail in a three dimensional format without possible damage to the sample. Computed microtomography and confocal microscopy offer non-invasive techniques that, after reconstruction of the data through computer programs, produce three-dimensional images of the insect that can reveal minute details of its anatomy. With this information, scientists such as entomologists, geologists, and paleontologists can infer statistics such as diet, evolution, and environmental characteristics of the insects and their surrounding biomes. Computed microtomography uses x-ray beams to perform scans on these samples at desired energy levels while confocal microscopy uses laser scans to obtain data. It is difficult to find the optimum energies to perform the x-ray scan on the amber because of its relatively low density and the fact that it and the insects share similar densities. The difficulties of confocal microscopy occur when trying to determine a wavelength that renders the amber "invisible" and allows only the insect to fluoresce. Both processes require small samples at thicknesses around 3000 microns or less to provide the best resolution.

Development of a Genetic Framework Map in Panicum virgatum. EMILY STAFFORD (University of North Alabama, Florence, AL 35630) LEE E GUNTER (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

An increasing consciousness of societal costs of the overuse of fossil fuels and the limitations in oil supplies has led to the consideration of alternative energy sources. The search for more ecologically sound and sustainable sources of energy has caused an interest in the development of a fast-growing native prairie grass: switchgrass (*Panicum virgatum*). The ultimate goal is to improve the biomass yield and feedstock quality of switchgrass to make it competitive as an alternative biofuel. The construction of a genetic framework map, used for quantitative trait loci analysis and detection, can help in obtaining this goal. Microsatellite marker loci developed for this project were selected to exhibit maximum polymorphism between the two parents of an intra-specific hybrid F1 family. Synthetic oligonucleotide primers amplifying these 20 loci were tested on 45 F1 progeny through DNA amplification, gel electrophoresis and fluorescent genotyping. Alleles present in one parent, absent in the other and exhibiting a one to one segregation ratio were used in mapping. After the initial testing of these twenty loci, ten produced alleles that were determined to exhibit the desired segregation. It is anticipated that approximately 130 evenly distributed markers will be required to create a useful map. Additional microsatellite markers need to be tested in order to complete construction of a full coverage genetic framework map.

Deployment of Phytoremediation at 317/319. SHEILA STOCK (College of the Redwoods, Eureka, CA 95501) M. CRISTINA NEGRÍ (Argonne National Laboratory, Argonne, IL 60439). Phytoremediation is the use of living plants to remove and/or degrade contaminated soil and groundwater. The Phytoremediation process acts as a system of treatment mechanisms that can include some or all of the following: sequestration, removal, stabilization, degradation, and mineralization. The 317/319 areas are on the southern end of ANL-E. This area was used to dump different types of solid and liquid wastes before 1980. In June of 1999, there were over 800 hybrid poplars and hybrid willows planted in the 317/319 areas. My research is to gather transpiration samples from leaves, perform methanol extractions and root washing on soil, and monitor sap flow to test for tritium and various volatile organic compounds (VOCs). Unfortunately, there will

be no results for this year because of the time it takes to run tests, at an outside lab, and the time I was here and able to gather testing materials. This project is not expected to end until at least five to ten years from now.

Correlating the Organic Composition of Corn to the Uptake of Lead From Soil. JYOTI TIBREWALA (*Massachusetts Institute of Technology, Cambridge, MA 02139*) LISA M. MILLER (*Brookhaven National Laboratory, Upton, NY 11973*).

The natural tendency of plants to extract heavy metals from soil is of great interest to scientists because phytoremediation represents an environmentally friendly way to clean up contaminated soil. In this work, synchrotron-based x-ray and infrared spectroscopies were used to examine the organic components of the corn plant, as well as the localization of lead taken up by the plant, in an effort to determine why corn has an affinity for lead. Lignin was isolated from corn stems, and infrared spectroscopy was used to characterize the various plant components. Corn plants were grown in lead nitrate, and x-ray microscopy was used to determine the localization of lead in the stem and root. After 18 days of exposure to 2 mM lead, the corn plants had >12 times more lead in the roots and >5 times more lead in the stem than baseline. Infrared imaging was used to map the organic composition of the stem and root. Cellulose was found to be uniformly distributed throughout the roots and stems. Conversely, lignin was found to be concentrated near vascular bundles (xylem and phloem). From x-ray imaging, lead was found in high concentration throughout the root, including a "hot spot" that may be a lead precipitate in the sample. In the stem, lead was found to be concentrated near the vascular bundles, co-localized with high lignin concentrations. This combination of x-ray and infrared microspectroscopies showed the correlation between lead and the organic plant components. Results from this research will be important for understanding why corn plants are efficient at extracting lead from the soil and may lead to the improvement in phytoremediation of contaminated soils.

Study of Natural Attenuation in New York/New Jersey.

LIZABETH TROCHE (*University of Puerto Rico, Cayey, PR 00736*). KEITH JONES (*Brookhaven National Laboratory, Upton, NY 11973*).

The NY/NJ Harbor contains a wide range of chemical contaminants. The origin of these contaminants is due to industrial and anthropogenic activities. Contaminated sediments affect the benthic organisms killing them and reducing the food available to larger animals. Natural attenuation uses naturally occurring processes to clean up sites, is non-invasive and allows the site to be put to productive use while being cleaned up, but requires carefully controlled conditions and monitoring of contaminant levels. SRB use sulfate as the oxidizing agent, the sulfate then is reduced to sulfide, which is a strong complex of heavy metals and creates a low redox habitat. The purpose of this experiment was to evaluate the rate of natural attenuation for organic compounds under different conditions of electron and donor acceptors favorable for SRB in NY/NJ Harbor Sediments. Several techniques were used to determine the attenuation of organic compounds and the immobilization of heavy metals. One is the FTIR-Spectra used to determine changes in organics composition. BIOMET technique used to test the bioavailability of the heavy metals and the toxicity of the sediment and MPN-test used to determine the presence of SBR. Although natural attenuation is a process that will take several months, even under the most favorable conditions, the initial results indicate the presence and activity of the endogenous SRB, a decrease in the organic contaminants, demonstrated by FTIR-spectra and the bioavailability of Zn was strongly reduced as compared to a reference sample. Therefore we conclude that natural attenuation of the harbor sediment can be a cost-efficient method for sediment conditioning.

Solubility of TCE in Aqueous Biomass Systems. CHRISTOPHER VODRASKA (*Whitman College, Walla Walla, WA 99362*) JOHN BARTON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Trichloroethene (TCE) is the leading groundwater contaminant in the country, due in part to its widespread use as an industrial solvent. In order to effectively model the fate of TCE in aquifers and vadose zones, partitioning data such as the maximum solubility and Henry's law constant for TCE must be known. Literature values for TCE solubility and Henry's law constant in pure water vary greatly. Solubility data range from 5 to 15 mM, while values for Henry's law range from 0.006 to 0.02 atm m³ mol⁻¹. It was found that the presence of biomass impacts the solubility of TCE in water by at least up to 2

orders of magnitude for whole yeast cells. In this study, equilibrium vessels were constructed to measure the parameters for TCE in pure water as well as the parameters for several different "fractions" of yeast isolated through differential centrifugation: cytosol, membrane, and cell wall/insoluble fractions. The solubility of TCE in pure water systems was experimentally found to be 7.58 - 1.14 mM, but, for instance, in a system containing 0.035 g cytosol mL⁻¹, the solubility increased by 1.3 orders of magnitude. Solubility generally increased linearly in relation to the biomass concentration of all three fractions examined. The Henry's law constant was 0.0100 - 0.0027 atm m³ mol⁻¹ for pure water, but at the above cytosol concentration, the value was 1.3 orders of magnitude less. Work is underway to include these data in a mathematical model to predict partitioning values for TCE in aqueous biomass.

Correlation and Source of Compositional Variation in the Member of Sentinel Bluffs, Columbia River Basalt Group.

VALERIE WHEELER (*Allan Hancock Community College, Santa Maria, CA 93454*) STEPHEN REIDEL (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The member of Sentinel Bluffs (SB) is one of many flow units that make up the Columbia River Basalt Group (CRBG). Terrestrial flood basalts like the CRBG are a type of large igneous province (LIP) consisting of massive outpourings of extrusive basalts and associated intrusive rocks. Characteristics of extrusive lava flows include vesicular flow tops and bottoms, which are typically both porous and permeable. Due to SB's vast areal extent and volume, along with optimum physical and chemical properties, it has been examined as a candidate for "geologic sequestration of anthropogenic CO₂". The chemical composition of basalt makes it ideal to react, under proper conditions, with gaseous CO₂ in order to form stable, and therefore, more desirable minerals. Correlation of major and trace elements throughout enables recognition of these lava flows across the Columbia Plateau. Identification of trends and relationships between elements will help make reasonable predictions of possible chemical reactions with CO₂. Size, lateral continuity, chemistry of the flows and chemical variations within the flows are examined by visual inspection and chemical correlations of borehole chemical analyses. The source of variation within the SB was found, in part, to be the result of mixing of two distinct chemistries. However, not all of the variations can be explained in this manner. Other processes modifying the chemistry probably include crystal fractionation and magmatic differentiation. Further studies into these processes and other possible speculations could be conducted utilizing complex modeling programs.

Effects of Meteorological Factors on *Colias philodice/eurytheme*, *Danaus plexippus*, *Pieris rapae*, and *Speyeria cybele* Activity. STEFANIE WILLIAMS (*University of Illinois - Chicago, Chicago, IL 60680*) RODNEY WALTON (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

It is considered that temperature has an effect on butterfly activity. Increased temperature yields an increase in butterfly activity. The purpose of this research was to find a relationship between butterfly activity and various other meteorological factors. I observed four species of butterflies; *Colias philodice/eurytheme*, *Danaus plexippus*, *Pieris rapae* and *Speyeria cybele*, during varying degrees of temperature, relative humidity and barometric pressure. A Pollard Walk transect was used to devise a route for observing and counting butterfly activity. The temperature, relative humidity and barometric pressure were recorded for each observation. At the end of the research, it was revealed that temperature was the ultimate factor underlying butterfly activity. Relative humidity negatively affected the activity of all four species while barometric pressure had a positive effect on butterfly activity. However, relative humidity and barometric pressure were likely to have correlated with temperature and therefore they were not as significant a factor as temperature. Of the four species, two (*Speyeria cybele* and *Danaus plexippus*) were low in abundance. This may have biased some results as there were far fewer data points for these species.

Evaluation of Indoor Concentrations from Outdoor Source Hazardous Air Pollutants. WAZIRA WITHERS (*Tuskegee University, Tuskegee, AL 36088*) BRETT C. SINGER (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The purpose of this research was to enhance the ability to determine how much of a particular set of hazardous air pollutants (HAP's) adsorb and desorb to and from typical indoor surfaces and the rates

at which this is occurring. The method used was GC/MS, Gas Chromatography/ Mass Spectrometry. GC/MS is a compilation of devices that together separates and quantifies selected compounds. According to CG/MS the pure compounds (injected at the start of the experiment) over time were being removed from the air and then re-emitted. The hypothesis was that dependent on ventilation there is a significant potential human health risk once compounds have entered a residence. However, further studies must be conducted to be conclusive.

Energy Efficient Lighting - Optics, Controlled, and Prototyping.

YONG YANG (Pasadena City College, Pasadena, CA 91106)

MICHAEL SIMINOVITCH (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Energy efficient, low glare, and adjustable lighting plays a major role in office illumination. The Berkeley Lamp is able to provide separate, controllable light sources for both the ambient and direct lighting components in one movable unit that allows a broad range of configurations for different tasks and saves energy by reducing unnecessary illumination. However, the Berkeley Lamp projects most of its intense direct light on a limited working plane. The floor lamp can free up working space and give a relatively more uniform distribution. Prototype 1 has been built; an intense glare from direct light component was discovered. Prototype 2 and 3 were built with diffuser and Miro reflectors to eliminate glare and reduce light loss. Intensity distribution and luminous flux of prototype 2 and 3 have been calculated using goniophotometer and compared with Berkeley Lamp. A luminance comparison between prototype 3 and Berkeley Lamp has been analyzed. Prototype 2 decreased intensity output and luminous flux, but successfully reduced glare. Prototype 3 has reduced the glare and also partially recovered light loss. The optical design of prototypes shows that floor lamp can be an effective and energy efficient office luminaire.

GENERAL SCIENCES

Instruction Manual for a Cosmic Ray Detector. MICHAEL

COLLIER (New Mexico Institute of Mining and Technology, Socorro, NM 87801) HOWARD MATIS (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

This summer, I wrote an instruction manual on how to build a cosmic ray detector. The detector is an educational outreach program for high school students that my mentor has developed. The detector's purpose is to enhance students' study of cosmic rays and nuclear science. Currently, students and faculty must build their own detector. My task was to write an understandable manual for them. I have completed the manual and am waiting for feedback on its effectiveness.

The Iridium Anomaly at the Cretaceous-Tertiary Boundary.

RYAN DUNNING (California State University Fresno, Fresno, CA 93728) FRANK ASARO (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Twenty years after its inception, the Asteroid (or Comet) Impact Hypothesis is the most widely accepted hypothesis regarding the mass extinction of species that marks the Cretaceous-Tertiary (K-T) boundary. Evidence for the impact is the high level of iridium found world-wide in the sediment layer that divides the Cretaceous and Tertiary geological periods. Use of neutron activation analysis (NAA) allows very sensitive measurements of iridium and very precise measurements of other element abundances. Continued analysis of the K-T boundary sediments is the subject of this report. Graphs are shown of element analysis of boundary samples at four different locations in the U.S. which confirm the iridium anomaly in the manner seen at previous sites. However, analysis of one of these sites in Colorado showed a significant amount of Iridium below the K-T boundary — well into the Cretaceous rock layer. The cause of this is unknown at the present time.

Analysis of WWII German Kernphysik Program Uranium Cubes for Possible Verification of DOE Uranium Sample. CATHERINE

GOFF (Massachusetts Institute of Technology, Cambridge, MA 02139) ERIC SMITH (Pacific Northwest National Laboratory, Richland, WA 99352).

Unlike the United States' Manhattan Project, the WWII German

Kernphysik (Nuclear Physics) program was never able to produce a critical nuclear reactor, despite many attempts by physicists Werner Heisenberg and Kurt Diebner. At the end of the war, an Allied fact-finding mission captured the subcritical uranium piles and sent them to the United States, where, fifty years later, one of the uranium elements supposedly ended up at the DOE headquarters. In an attempt to verify this uranium cube's origin, historical information on the chemical and physical attributes of the German cubes was compiled. The cubes, of documented size and density, consisted of unenriched uranium, which could easily be determined in the sample through nondestructive gamma spectroscopy. Presence of an anti-corrosive, fission/activation products, or aluminum could also be determined by nondestructive methods, and would provide further evidence that the cube was of German origin. High-resolution gamma spectroscopy based solely on the relative concentrations of uranium decay chain daughters was examined as a dating method through computer simulation, but appears to be ineffective in dating a sample of this age. However, mass spectrometry is an option that uses a minimal sample and physically measures amounts of natural decay products to reliably date uranium.

Development of a Code for Studying Anisotropic Elasticity.

LARA C. JOHNSON (Presbyterian College, Clinton, SC 29325) LEN GRAY (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Computational analysis is effective for studying materials, and the Boundary Element Method (BEM) is often used for solving problems in linear elasticity. This method can easily be applied to materials that are isotropic. However, things become more difficult when working with materials that are anisotropic. The basis of the BEM is knowing a Green's Function (GF), or fundamental solution, and for anisotropic materials this function cannot be written in simple closed form. The GF is singular, and in the BEM it is necessary to exactly integrate the singularity. Lacking a closed form considerably complicates the analytical evaluation. We have developed methods for analyzing these anisotropic singular integrals, not only for the GF, but also for the more singular integrals involving its derivatives. A symbolic manipulation program, Maple, was used to evaluate the integrals and produce the needed Fortran code. With the singular integrals evaluated, the FORTRAN code for solving elasticity problems can be completed. With this new code, studies of anisotropic materials, especially crack propagation, can be carried out.

A Preliminary Economic Analysis of Tradable Credits for Fuel Economy Standards. SANJANA AHMAD (University of Tennessee, Knoxville, TN 37996) DAVID L. GREENE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Passenger cars and light trucks account for 40 percent of U.S. petroleum consumption and 20 percent of U.S. carbon dioxide emissions. Increasing the fuel economy of passenger vehicles is thus a critical strategy for reducing greenhouse gas emissions and dependence on oil. Since 1975, fuel economy has been regulated by the Corporate Average Fuel Economy (CAFE) system. The National Research Council, in a study on the impacts of CAFE standards, noted that, "other policies could accomplish the same end at lower cost, provide more flexibility to manufacturers, or address inequities arising from the present system." A possible alternative "tradable fuel economy credits system" was considered particularly attractive. Tradable credits have successfully been used to reduce sulfur dioxide emissions from power plants. This paper presents an initial assessment of the economic efficiency of a tradable fuel economy credits system, its impacts on manufacturers and the structure of the credits market. The problem is formulated as an optimization model where the net value of fuel economy increases is maximized subject to the fuel economy standards and credit constraints. Results indicate that tradable credits are more economically efficient than the current approach, but the competitiveness of the credit markets is uncertain. Both the buyer and seller markets are likely to be highly oligopolistic, raising doubts about whether the efficiency gains of the tradable credit system could actually be realized. A tradable credit system will probably result in substantial transfer payments among a few manufacturers, raising questions about the political viability of such a system.

Current Practice, Code Compliance and Enforcement Data Set.

JOHN GRAY (Bucknell University, Lewisburg, PA 17837) DIANA SHANKLE (Pacific Northwest National Laboratory, Richland, WA 99352).

Building energy codes are established to help consumers save money, the nation to conserve its national resources, and the environment to remain unpolluted for future generations. Prior attempts to analyze the effectiveness of energy codes contained assumptions regarding specific types of data that have the potential to affect the accuracy of conclusions drawn from it. Through in-depth data mining, networking, and surveying, a greater breadth of information has been gathered in order to put real numbers behind many of these assumptions, and to grasp past successes and chances for future savings with more accuracy and detail. This was accomplished by gathering data on the state, instead of national level, and through surveying state code officials, gathering estimates of compliance levels and enforcement practice. In the end, spreadsheets were produced containing data on current and historic population, building starts, energy consumption and prices, and energy code legislation changes, and code adoption and compliance rates at the state level. This information will help in providing accurate measurements of past savings, as well as serve as baseline data for inquiries into estimated future savings.

Family Health Curriculum Development. AMANDA KNUDSON (*Northwestern University, Evanston, IL 60208*) KATHY BARRETT and MARY CONNOLLY (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Health is of utmost importance within the family unit. The first step toward a healthy family is learning about ways to keep healthy. A current method of teaching families about some of the health risks they face is through outreach programs. Building on previous work, extensions were made into asthma, hepatitis, and nutrition. Using background research, public trials, and integration of feedback, family health educational curricula evolved. The existing asthma module was updated to concentrate the focus more on learning to control one's breathing. The hepatitis module was unprecedented and was developed for teachers to explore the spreading of hepatitis A and B through classroom activities. The existing nutrition modules were extended so as to include fat and fiber. The modules developed show promise toward educating families about important health issues.

Development of an In-situ Flow Through Photoacoustic Sensor. MICHAEL LOW (*University of Nevada, Reno, Reno, NV 89503*) THOMAS AUTREY (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The ability to detect small concentrations of chemicals in solution is of great importance to scientists in environmental, pharmaceutical, and other areas research. Development of a flow through photoacoustic sensor will advance the in-situ detection methods currently available. The increased sensitivity of photoacoustic spectroscopy and the layered prism cell (LPC) provide a solid basis for improved detection. With degassed water flowing through the LPC, 200 μL injections of Acetaminophen (concentrations ranging from 2.67 μM to 8.2 mM) were injected into the cell. Direct comparison of the resulting photoacoustic signals obtained with a pulsed xenon flash lamp with those obtained by a UV-Vis absorbance detector show that the photoacoustic sensor does not provide better detection as we initially expected. However, more research is needed to maximize the detection capability of the flow through photoacoustic sensor. Our initial results and suggestions on improving the sensitivity of the photoacoustic sensor are presented.

Mankind and the Balance of Nature. LISA POLONSKI (*Marist College, Poughkeepsie, NY 12601*) and DEBORAH SIMS (*California State University, Northridge, Northridge, CA 91330*) GAIL DONOGHUE (*Brookhaven National Laboratory, Upton, NY 11973*).

Man has not always been respectful of his surroundings; he continues to leave scars on the natural habitat. Destruction of the rainforest, erosion of our coastlines, and pollution in our cities are all examples of the negative impact of mankind. Through the education of students at a young age, this situation can be reversed for the better. The importance of integrating environmental issues to other areas of the curriculum has been lagging in our schools. It is the goal of this project to integrate environmental science across the curriculum to formulate a better understanding of mankind's place as it relates to his/her environment. To accomplish this goal, students will be taught lessons on the ecosystem and mankind's relationship with nature, concentrating on five areas: trees, soil, animals, habitats, and the environment. We will show how each is dependent upon the other for survival. Assessment will be accomplished by having students write journals,

create visual art, read related literature, utilize problem-solving techniques, and participate in scientific inquiry. This enhanced understanding of nature and the delicate balance between it and mankind leads to better choices, which in turn will enable students to make a difference in the world around them.

Documenting Procedures at the Institute for Superconducting RF Science and Technology. KATHERINE SHOWALTER (*James Madison University, Harrisonburg, VA 22657*) CHARLES REECE (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

The Institute for Superconducting RF Science and Technology uses DocuShare software to document, store and retrieve the information generated during actual procedures as they are done. The DocuShare system uses documents called "travelers" to capture the data. A proposed link between the traveler document and the common procedure document would provide a complete document package. Common procedures integrated within the Traveler documents will enhance productivity and facilitate the virtual cross-functional intent of the work allowing other members of the collaboration access to the data. This access will allow off site members of the SNS collaboration the ability to electronically interface with members here at Jefferson and the other laboratories.

MATERIALS SCIENCES

Testing the Theoretical Prediction for Coherent Vortex Flow in Layered High-Temperature Superconductors. JEREMIAH S. MCNATT (*The University of Akron, Akron, OH 44325*) PETER BERGHUIS (*Argonne National Laboratory, Argonne, IL 60439*).

Preparations are made with the desire to test the theory of coherent vortex flow in high-Tc superconductors. In this paper we explain the setup of the environment needed for such an experiment: we show that gold, quartz, and BISCO have similar enough thermal expansion rates to be used together and we give details on a sample holder and a high precision tool to align superconducting crystals with external contacts. This work shows the preliminary steps being completed before testing our theory. Future work will test both theory and our newly designed equipment.

Melt-loss Project. JESSICA ANDERSON (*Iowa State University, Ames, IA 50011*) GREG KRUMDICK (*Argonne National Laboratory, Argonne, IL 60439*).

The aluminum manufacturing and recycling processes in industry are of large concern to aluminum companies and energy conservationists. In industry, the process of melting aluminum is crude and inefficient leading to gross amounts of waste product from which the aluminum cannot be recovered. Also, due to this melting process, a great deal thermal energy is wasted in an effort to heat the aluminum through its dross (or oxide) layer that has a higher thermal capacitance than aluminum. Therefore, it is desired to lessen or eliminate the amount of dross growth on molten aluminum to reduce waste and also diminish the energy needed to keep the aluminum in the molten state. Until recently, aluminum melt dross formation and its thermal properties were not well understood. Only a few crude methods of controlling the dross formation existed and often resulted in contamination of the melt. A new method of controlling dross formation is being researched which involves a melt cover of a higher thermal capacitance than the dross layer that is not attacked by molten aluminum. Preliminary results of this new method are successful. Using techniques such as temperature profiling and mass assessments of the melt to compare the amount and type of dross formation, the results show that this cover has reduced the amount of dross formation by a significant amount.

Temperature Calibration of High Temperature X-ray Diffractometers Using Thermal Expansion Standards. REGINA BRYSON (*Motlow State Community College, Lynchburg, TN 37352*) E. ANDREW PAYZANT (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

High temperature X-ray diffraction (HTXRD) is increasingly being used as a routine characterization technique. This necessitates the development of procedures to ensure accurate temperature calibration. Temperature calibration curves produced with external standards may not compensate for the specific nature of a sample. Therefore, this study explores the use of potential internal standard materials with

well-characterized thermal expansion coefficients that can be used to calibrate temperature. So that a standard appropriate to the sample can be chosen, a selection of potential HTXRD standards was qualified. Appropriate standards should not react with the sample or the holder on which they are placed; should be nonvolatile, that is not evaporate or melt in the temperature range used; should have minimal overlapping with the peaks of the sample; and be readily available and inexpensive. The powders used in this stage of the research were magnesium oxide (MgO) and zinc oxide (ZnO). Since standards need to be independent of the instrument used, calibration data were collected on diffractometers with different furnace designs and beam geometries in order to avoid machine-specific artifacts. Also, several methods were utilized in analyzing the data to determine consistency. To test the accuracy of temperature calibration, the standards were subsequently mixed and examined with a deliberate thermal offset error. These standards prove a viable method of calibration with the proper considerations given to the material being characterized. Further research will be done in qualifying other standards.

Biomedical Applications of Thermoreversible Gels. *YOUNG-ME CHUNG (University of California, Berkeley, Berkeley, CA 94720) ANNA GUTOWSKA (Pacific Northwest National Laboratory, Richland, WA 99352).*

The feasibility of using thermoreversible gels for two biomedical applications, drug delivery and micropatterning, was investigated. For the drug delivery application, aqueous solutions of copolymer poly(DL-lactic-co-glycolic acid)-g-poly(ethylene glycol) (PLGA-g-PEG) with additives were characterized in terms of sol-gel transition temperature, mechanical strength, in vitro degradation, and additive release. For the micropatterning application, aqueous solutions of thermoreversible gels homopolymer N-isopropyl acryl amide (NiPAAm), collagen, and agarose were micropatterned into channel and square-grid structures with varying success. The composition of PLGA-g-PEG solutions as well as the techniques and characterization for micropatterning NiPAAm, collagen, and agarose require additional development. Eventually, large-scale in vivo studies using PLGA-g-PEG as an injectable drug delivery system and cell development and tissue engineering studies using micropatterned gels may be conducted with optimized polymer formulations.

Using Sizing to Improve the Interfacial Strength of Composites. *AMANDA CLAUSEN (Pima Community College, Tucson, AZ 85730) KEVIN SIMMONS (Pacific Northwest National Laboratory, Richland, WA 99352).*

There is always a push in our society to find a way to make things lighter, cheaper, and stronger. Thus, making fiberglass composites stronger has been an on going area of research for years. Studies on composites have shown that if the interfacial bonding between the phases of the composite is improved then the overall strength and durability of the composite increases. Before the glass was impregnated with resin, layered, and pressed into panels, the glass was treated with a fiber sizing to increase the interfacial adhesion capabilities of the glass to the resin. Test panels were made with untreated glass, glass treated with a commercial sizing, sizing A, or sizing B. These panels were then tested for tensile, flexural, and shear strength. Results show that the panels made with the glass treated with the sizing A and B significantly increased the strength of the composite compared to the untreated glass panels. The physical properties of the panels made with the glass treated with the sizing A and B rival those of the panels made with the glass treated with the current commercial sizing, but do not show a drastic increase in strength as expected. Methods for further testing of other physicals properties and sizing agents are under consideration.

Novel Oxide Catalysts. *JANELLE CRITCHFIELD (University of Washington, Seattle, WA 98195) JENNIFER MAWDSLEY (Argonne National Laboratory, Argonne, IL 60439).*

Fuel cells operate at a higher efficiency with less noise than the internal combustion engine in transportation applications. Although fuel cell technology is appealing on paper, the ability to harness the electrical energy from hydrogen and oxygen is challenging. For this summer project, autothermal processing is the primary reaction to produce hydrogen from liquid hydrocarbon fuel by using novel oxide catalysts in a microreactor. The catalysts synthesized had the perovskite formula ABO_3 . The previously tested catalyst $LaCr_{0.9}Ni_{0.1}O_3$ performed well, and new catalysts were synthesized with variations

of this formula by substituting or doping rare earth elements, alkaline earth elements, and transition metals. The results included for this report take place at 700 °C at various gas hourly space velocities (GHSV) and at 4655 hr⁻¹ for various temperatures. It was seen that the hydrogen production decreases with increasing space velocity for all catalyst compounds. This trend is expected due to the decrease in contact time between the catalyst and reactants. Doping the catalysts has negative effects on hydrogen production at low space velocities.

Nonconsumable Inert Anode for Aluminum Electrolysis. *SOM DAS (University of Illinois, Urbana Champaign, IL 61820) JIANHONG YANG (Argonne National Laboratory, Argonne, IL 60439).*

High-energy consumption, environmental pollutants, and high cost in the current Hall-Héroult process for aluminum production, necessitates the development of a non-consumable inert anode for the electrolytic processing of alumina to aluminum. A copper based metal anode shows promising signs of a non-consumable anode. Commercially available copper and copper alloys were used in conjunction with varying the fluoride electrolyte composition in order to find a viable non-consumable anode. Copper alloys were made for future anode material consisting of aluminum, copper, and/or silver in order to find a viable non-consumable anode using an electric furnace in an inert argon atmosphere. The non-consumable anode must form a uniform and thermally stable oxide layer to prevent the base metal from further reacting and dissolving into the fluoride electrolyte bath and to resist thermal shock. In order to understand the behavior of the oxide layer, the copper anode materials are oxidized in an electric furnace at 710°C. Pure copper samples show to follow a parabolic oxidation curve as expected.

Hydrogen and Oxygen Diffusion and Oxygen Sensing Using YSZ Probe. *SAM DONALDSON (University of Illinois, Urbana-Champaign, Urbana-Champaign, IL 61801) JONG-HEE PARK (Argonne National Laboratory, Argonne, IL 60439).*

Using an yttria-stabilized zirconia, oxygen ion conducting probe in a gas tight system, we monitored the rate of diffusion of hydrogen and oxygen through a thin silver membrane. Steam dissociates and permeates through a membrane at elevated temperatures.

How Changing the Precursor and Heating Rate Affects Physical Properties of Carbon Foam. *CAMERON DRUMMOND (Cornell University, Ithaca, NY 14853) NIDIA GALLEG0 (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

Carbon foam recently developed at Oak Ridge National Laboratories has many uses pertinent to the Department of Energy's goals. It has potential in heat exchangers and self cooling-devices among other things. The foam has already proven itself as a capable lightweight alternative to the heat exchangers in existence today. At this point in research the foam is being refined in order to obtain a final product that is most capable of performing such tasks. In the quest to make a foam with maximum utilization, the way in which the foam is made is being varied, which in turn changes the physical properties of the foam. Two mesophase pitch batches were made by Conoco, batch A and B respectively. Two heating rates were used as well creating a matrix that can easily be analyzed in order to determine the samples created with the most distinguishing characteristics. The heating rates were 1.0 Co/min and 3.5 Co/min during the foaming process, rates A and B respectively. Sample 190-4, which used Precursor B and Heating Rate A proved to be the most thermally and electrically conductive, as well as being the most uniform. Previous studies have shown that the thermal conductivity of the sample has increased linearly with density and the data acquired in this experiment confirms these presuppositions. It can be shown from the data acquired that by varying the precursor and heating rate during the foaming process, one can modify the physical properties of the foam, tailoring it in order to produce a product with desired characteristics.

Pulse Brazing of 6061 Aluminum. *JERED FRY (South Dakota School of Mines & Technology, Rapid City, SD 57701) CRAIG A. BLUE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

Ford Motor Company is considering the use of 6061 aluminum alloy for automotive body panels. However, due to aluminum's high affinity for oxygen, it is difficult to fuse aluminum materials by conventional welding. A prospective method for joining such panels employs ultrasonic spot welding to hold panels in place, followed by the use of a high-density infrared (HDI) source to braze them together. Ford is

cooperating with Oak Ridge National Laboratory to investigate the use of ORNL's 300 kW plasma lamp as the HDI source. Initial experiments were performed in a highly controlled 33 kW infrared (IR) furnace to observe interfacial phenomena as a function of time, temperature, and fluxing agent. Specimens consisted of uniform weight samples of flux core or solid braze on 1.0 cm² by 0.093 cm thick samples of 6061 aluminum. Experiments with the IR furnace showed longer ramp times (fifteen to thirty minutes) and low temperatures (450°C to 475°C) yielded a large amount of porosity throughout the braze and at the interface. Better wetting occurred at shorter times and higher temperatures (>490°C). Ramp times less than one minute returned best results. Several experiments using the plasma lamp at a peak power density of 330 W/cm² show excellent interfaces. Experiments for 2.54 cm by 7.62 cm samples, electrically spot welded from the same material, were generally unsuccessful with the plasma lamp. However, ultrasonically spotted samples supplied by Ford worked extremely well due to their superior contact and subsequent heat transfer. Mechanical testing proved the joints were high-quality.

Novel X-Ray Zone Plate Design Evaluation using Visible Light Model. AYISHA FULLERTON (Norfolk State University, Norfolk, VA 23504) ALEXANDER LIDDLE (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The zone plate has been essential to the advancement of X-Ray microscopy. Zone plates are used to focus X-Rays because, unlike optical microscopes, effective refractive lenses do not exist. The purposes of this research include designing and constructing a visible light analogue of the X-Ray microscope at LBNL for testing and educational purposes, and enabling the exploration of some novel zone plate concepts, such as a photon sieve. Currently, the XM-1 at LBL can resolve features as small as 25nm. However, novel zone plate designs that relax the fabrication requirements are predicted to resolve features twice as small. The resolution of the X-Ray microscope is dependent on the wavelength of the light and the numerical aperture. In conventional zone plates the numerical aperture is dependent on the width of the outermost zone of the zone plate, which is limited by the fabrication process. Currently, the XM-1 at LBL can resolve features as small as 25nm. An important goal of the research is to decouple the dependency of the numerical aperture to the width of the outermost zone using these novel zone plate designs. Results for different designs are obtained from this research so that the most effective designs can be implemented to improve the resolution of the X-Ray microscope at LBL.

Generating, Detecting, and Analyzing High Frequency Acoustic Signals in Accelerator-Grade Copper. ELIZABETH GREEN-WOOD (Massachusetts Institute of Technology, Cambridge, MA 02139) JOSEF FRISCH (Stanford Linear Accelerator Center, Stanford, CA 94025).

One of the major limitations on the Next Linear Collider (NLC), a high-gradient particle accelerator in development, is that sparks form within the copper structure, damaging the material. The sparks also generate high frequency acoustic signals that can be used as diagnostics to solve the problem. First, however, the signals' location, attenuation, and propagation must be established, so an effective method for generating and detecting these signals in a simple copper block is necessary. Impact trials with ball bearings and a BB gun as well as tests with a grinder, a laser, and a sparker were conducted to determine how to produce the greatest ratio of high to low frequency acoustic signals. The laser had the largest ratio, but the sparker was chosen because it also had high ratios and was both more practical and more analogous to the actual signals in the accelerator. Further tests were then conducted to determine the best sensor; an International Transducer Corporation 9020 1 was chosen. Subsequent analysis of signals using this setup could establish the location and types of signals and, ultimately, how to solve the problem in the structure.

Development of an Environmentally Friendly Deicing Fluid. LIBBY HEEB (University of Washington, Seattle, WA 98195) BILL SAMUELS (Pacific Northwest National Laboratory, Richland, WA 99352).

Ethylene and propylene glycols, both of which are toxic to humans and other animals, are currently the standard deicing fluids for military and commercial aircraft around the world. There is a great need for biofriendly alternatives to these fluids. Solutions similar to a glycerol

based deicing fluid that had already been certified for use by the aviation community were studied for viscosity, thermostability, freezing point, and solubility properties. Several solutions studied have potential to be certifiable. However, in the future more tests must be performed on the candidates before certification is possible.

Growth Studies of Gadolinium Zirconium Oxide (Ga₂Zr₂O₇) Thin Films on Textured Ni-Substrates using a Solution Process for High Temperature Superconductors. PETER HELLENBRAND (University of Wisconsin-Madison, Madison, WI 53706) M. PARANS PARANTHAMAN (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

A low cost, non-vacuum, solution process was used to grow epitaxial Ga₂Zr₂O₇ (GZO) buffer layers on textured Ni (100) substrates for YBa₂Cu₃O_{7-y} (YBCO)-coated conductors. The GZO precursor solution was prepared by an alkoxide route using gadolinium acetate and zirconium n-proxide mixed in 2-methoxyethanol. The solution was spin-coated on short lengths of the textured Ni substrates. The coated tapes were heat treated at temperatures ranging from 1050-1200°C under Ar/H₂ (4%) atmosphere for 1 h. X-ray diffraction patterns of the GZO films revealed c-axis orientated growth. Scanning electron microscope images of the GZO layers show a dense and crack-free microstructure. Results of superconducting YBCO films deposited on the GZO buffered substrates by pulsed laser deposition will also be presented.

Preparation and Characterization of Superconducting Niobium Tips for Observation of Vortices with Scanning Tunneling Microscopy. MARY HUGHES (University of San Francisco, San Francisco, CA 94117) GORAN KARAPETROV (Argonne National Laboratory, Argonne, IL 60439).

In the past ten years, the scanning tunneling microscope (STM) has been used extensively to study magnetic flux vortices in type II superconducting samples. With the advent of successful fabrication of superconducting tips for the STM, it should now be possible to study the properties of vortices in the tips. To study these properties, it is important to control the shape, size and cleanliness of the tips. We report on an attempt to control these aspects of the tips. Tips were fabricated in two ways: by electrochemical etching in a standard buffered chemical polishing (BCP) solution and mechanical sharpening. For those made by etching, a correlation between the power applied to the tip during etching and the angle of the tip was found. Tips etched in the BCP solution were brittle and broke easily. Most tips did not show superconductivity, due to oxidation on tip surface. Attempts at observing vortices were not successful because of noise. The characteristics of a tip are very dependent on the exact conditions of fabrication. Further work needs to be done to control the etching process.

Process Analysis of Metallorganic Chemical Vapor Deposition of Yttria-Stabilized Zirconia Coatings for Thermal and Environmental Barriers. REBECCA HYDE (Mississippi State Technical Community College, Knoxville, TN 37933) THEODORE M. BESMANN (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Yttria-stabilized zirconia (YSZ) is a ceramic coating used to thermally insulate turbine blades in the high temperature corrosive environments of gas turbine engines. The current method of producing YSZ coatings, electron-beam physical vapor deposition (EB-PVD), can provide the desired columnar microstructure and deposition rate for YSZ coatings but is too expensive in production and operational costs. A less expensive alternative to EB-PVD is metallorganic chemical vapor deposition (MOCVD) that can be used to supplement or potentially replace EB-PVD. Although many factors affect the deposition rate and quality of YSZ coatings produced by the MOCVD reactor this investigation will focus on the effects of temperature between 500°C and 1000°C as well as the concentration of the precursors. Solubility experiments, using common industrial solvents and the two precursors were completed in an effort to increase the amount of reactants reaching the surface of the substrate in a definite time interval and eliminate the negative effects of excess solvent addition. Results regarding the temperature effect on YSZ coatings were monitored using X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM). It was found (1) an increase in coating thickness occurred with an increase in temperature and (2) tetrahydrofuran (THF) provided the best dissolution of both precursors. Future investigations of pressure and overall gas-flow rate effects in this MOCVD reactor on YSZ

coatings will be attempted to maximize deposition rate and achieve the desired columnar microstructure.

Silane Based Self-Assembled Monolayers on Silicon Wafers. JANA JACOBSON (*Montana State University, Bozeman, MT 59715*) WILLIAM D. SAMUELS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The purpose of this research was to ascertain synthesis conditions for acryloxypropyltrimethoxysilane (acryl si) and vinylbenzylmethylamidepropyltrimethoxysilane (vinylbenzyl) self-assembled monolayers. Once synthesized, ellipsometry measurements were performed to establish monolayer thickness (in angstroms). Static contact angle measurements were used to evaluate wetting properties, uniformity, surface-free energy, and information on surface order. Silicon wafers covered with the self-assembled monolayer should have a high contact angle due to the non-polar end groups of the silane compounds. Silicon wafers with approximately an 18-angstrom native oxide coating have a low static contact angle due to the hydrophilic property of hydroxyls. All monolayers displayed favorable results when synthesized thirty minutes at elevated temperature. Vinylbenzyl samples synthesized by first creating the silane then attempting to attach the compound to the silicon surface gave inconsistent results that did not match expected ellipsometry and static contact angle values. Vinylbenzyl monolayers must be synthesized stepwise, first attaching aminopropyltriethoxysilane (APS) to the silicon surface, and then 4-vinylbenzyl chloride to the APS monolayer.

The Effects of Aperture Dimensions Upon X-ray Image Contrast.

SARAH JAGODZINSKE (*North Park University, Chicago, IL 60625*) GREGORY DENBEAUX (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

XM-1 is a high-resolution, soft x-ray microscope, used for many types of scientific research. XM-1 is constantly striving to improve the quality of their images. A linear monochromator consisting of a fresnel zone plate and a pinhole gives us energy of a specific wavelength, determined by the distance between the two components. This setup does allow small percentages of unwanted energies. Our project this summer was to investigate the extent that light of unwanted energies affects our image quality. Calculations were done based on the chromatic aberration to determine what unwanted light gets through at different energies. We tested image contrast with the x-ray microscope by measuring unwanted light in images as a function of the illumination pinhole size. For the 17 micron pinhole one image contained 49.1% and the other 58.1% of light was present in the nominally dark region of our images. Images for 5 mm, 10 mm, and 20 mm pinholes were unable to be taken due to lack of beam time as well as an underestimated amount of time needed to complete the experiment. Therefore, comparisons of different pinhole sizes are unavailable, but we suspect that smaller pinholes will result in less unwanted light in our images, which will lead to better contrast and possibly higher resolution. Further investigation will continue at a later date.

X-Ray Computed Tomography Phantom Development. SARAH JANNEY (*University of Tennessee, Knoxville, Knoxville, TN 37916*) APRIL D. MCMILLAN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

X-Ray Computed Tomography (CT) is an imaging method used for disease diagnosis, to visualize internal 3D structures, and as an aid for planning surgical treatment. The CT detects small changes in physical properties, such as density or chemical composition. Therefore, it is used to detect small tumors and other irregularities in humans. Current CT phantoms used for testing need improvement to ensure that the CT reads well in three dimensions. A phantom is a part having objects of one material and density embedded in the same material with a different density ($\pm 1\%$ difference). Currently, no phantoms allow for contrast measurements in three dimensions, which would permit earlier detection of tumors and other irregularities. The phantom must simulate x-ray density of human internal organs, for which the material boron carbide (B4C) provides a good match. B4C, a ceramic, requires a ceramic forming process. Gelcasting, a slurry molding process developed by ORNL, was chosen to produce a 3D phantom in B4C. The phantom is then fired to achieve final densities. Difficulties were encountered in gelcasting B4C due to thickening of the slurry and premature gelation. Changing monomers produced a more fluid slurry that cast and gelled well. Phantoms should be 50% of theoretical density to simulate human tissue. Current densities are too high, near 60%. Modifying the solids loading of the slurry should yield the desired

density. The final phantom will be cast in layers with contrast objects of different density between the layers, creating a three-dimensional pattern. The end result will be a sintered phantom capable of reading in three dimensions.

Single Crystal Anisotropic Conductivity Measurements for $\text{La}_{2-2x}\text{Sr}_x\text{Mn}_2\text{O}_7$ at $x = 0.54$. BENJAMIN JARVIS (*Yale University, New Haven, CT 06520*) KENNETH GRAY (*Argonne National Laboratory, Argonne, IL 60439*).

Recent developments at Argonne National Lab have allowed for the production of single crystals of $\text{La}_{2-2x}\text{Sr}_x\text{Mn}_2\text{O}_7$ manganite at the $x = 0.54$ doping level. These crystals provide a new composition in which to explore the close interdependence of lattice, spin, charge, and orbital degrees of freedom in determining the complex magnetic characteristics of this class of materials. Using 6 and 8 terminal measurements, we attempt to find the anisotropic conductivity of a sample at this composition. We measure this conductivity as a function of temperature and magnetic field. Our measurements show behavior in opposition to those expected by theory. We suggest that these abnormalities result from an inhomogeneous sample.

UV Raman Spectroscopy of NFC's. WILL KING (*Purdue University, West Lafayette, IN 47906*) JACKIE JOHNSON (*Argonne National Laboratory, Argonne, IL 60439*).

In recent years there has been a scientific lean towards more extensive research on diamond-like carbon coats referred to as DLC's. DLC refers to any material containing multiple different carbon bonding structures anywhere from the simplest C-C bond to diamond sp³ bonding. Most recently the push here at Argonne in the Tribology Section of the Energy Technology Division has been to experiment with the process of making these coatings. Sputtering and plasma-enhanced chemical vapor deposition (CVD) are two processes that have been used to further enhance the quality of coatings that can be made. Using plasma-enhanced CVD a very low friction coating was discovered called near frictionless carbon (NFC). NFC's are unique to Argonne because they were discovered here in the Tribology section, and these coatings have friction coefficients ranging from .001 to .013 when tested in dry nitrogen or inert gas environments. The current push is to more closely investigate the structure of these NFC's in an attempt to characterize the internal bonding. Possible contributions to the extremely low coefficients of friction may be the ratio of diamond, sp³, to graphite, sp², bonds. I will be working with J.A. Johnson in an attempt to further characterize NFC coatings. We will be using a laser to do UV Raman spectroscopy of our samples in an attempt to extract curve fit data from the results. The laser lab is already set up, my major responsibility will be in curve fitting and data analysis. I will be documenting on how to properly fit UV Raman data from NFC's along with any results that I may find.

Microwave Heating for Pack Cementation Coatings. MARK LOSEGO (*Pennsylvania State University, University Park, PA 16802*) TERRY N. TIEGS (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Pack cementation is a widely used surface treatment method for metal components that need to withstand hostile environments or require augmented surface hardness. This research investigated the feasibility of using microwave (MW) heating during pack cementation in place of conventional conductive heating methods. Because of its cost-effectiveness and heat-transfer efficiency, the use of MW heating is a potentially advantageous process for industry. Three representative alloys were chosen for this investigation: a tool steel (A-2), a low carbon steel (1018), and a Ni-Cr alloy (625). Packing powder contained 83 wt.% Al_2O_3 , 2 wt.% NH_4Cl , and 15 wt.% of the source material. Two sources were studied: metallic aluminum and Cr_2O_3 . For each packing composition, two runs were made in the MW furnace—one at 850°C and the other at 925°C. These four runs were then duplicated in a conventional tube furnace. The size and weight of the samples were monitored for each run. Longitudinal sections of the samples were examined with optical microscopy, electron microscopy, and energy dispersive x-ray analysis. X-ray diffraction was also performed on the surfaces to help determine phases present. Aluminized samples showed thick reaction layers. The aluminized MW samples demonstrated unusual growth and diffusion kinetics along with compositional differences. Chromized samples exhibited a diffused coating with little reaction above the original surface. To some extent, data from the chromized steel samples indicated less diffusion and less uniformity in the MW group. Further work should focus on

determining the performance of these MW processed samples in corrosion tests.

The Effect of Montmorillonite Acidity on Etioporphyrin. *KALIKA LOW (Whitworth College, Spokane, WA 99251) NANCY FOSTER-MILLS (Pacific Northwest National Laboratory, Richland, WA 99352).* Clays become increasingly acidic as depth of burial increases and water content decreases. This acidity increase also increases the number of conversions of free-base and metalloporphyrin species sorbed on clay to the dication form. The ratios of etioporphyrins in the dication form to those not converted may provide information for locating plentiful petroleum sources. Various solvent/ acid combinations were explored to determine the best matrix; chloroform/ trichloroacetic acid was chosen. Extinction coefficients for porphyrins in chloroform were also determined. The change in acidity of montmorillonite clay as a function of water content was measured using diffuse reflection spectroscopy and Hammett indicators. As water content increased, the clays became more basic as was seen by a shift in the spectra. In this paper only copper, nickel, vanadyl and freebase etioporphyrins were researched, but other porphyrin species should be researched in the future.

Synthesis of Single Phase SrCu₂O₂ from Liquid Precursors. *ALEX MARTINSON (Luther College, Decorah, IA 52101) DAVID GINLEY (National Renewable Energy Laboratory, Golden, CO 89401).*

We report on the first successful non-vacuum deposition of single phase SrCu₂O₂ from liquid precursors by spray deposition as well as experiments on the deposition of SrCu₂O₂ thin films by inkjet printing. Liquid precursors for SrCu₂O₂ were made by dissolving copper formate and strontium acetate in water. Bulk single-phase powdered SrCu₂O₂ was synthesized through the spray deposition of liquid precursors at 180°C followed by a 4 hour anneal at 775°C and 2.0 x 10⁻⁵ Torr vacuum. Additionally, CaCO₃ was successfully added to the precursor solution above and subsequently incorporated after annealing. This was a critical demonstration of the ability to do cation substitutions by this approach. Employing the liquid precursor for thin films resulted in mixed phase SrCu₂O₂ and Cu₂O due to Sr loss during annealing. The liquid precursor was also successfully inkjet printed.

Synthesis, Structure, and Electrochemical Characterization Of Two Silver Copper Oxides: Potential New Cathodes for Implantable Medical Devices. *CRYSTAL MAY (Saint Mary-of-the-Woods College, Terre Haute, IN 47876) JOHN T. VAUGHNEY (Argonne National Laboratory, Argonne, IL 60439).*

Many devices exist today that require a better power source than is currently available. For medical applications, many of the current battery options are too heavy, do not provide enough power, or lose energy on extended storage (Alper, 2002). This study focuses primarily on compounds for intended use in implantable cardiac defibrillator (ICD) batteries. The primary (non-rechargeable) lithium batteries currently in use in ICD's provide adequate power and are able to sit unused for extended periods of time, but some lifetime problems have been identified that makes the introduction of other materials possible in order to defer the need for battery replacement surgery. Presently, silver vanadium oxides (SVO's) have proven to be both safe and reliable in ICD's, although the next generation of medical devices will need batteries that have a higher capacity with more stable performance over the whole voltage window. In our study we evaluated silver copper oxides (SCO's) as possible candidates for next-generation ICD's. Silver copper oxides in this study were synthesized using a low temperature and low-pressure procedure and incorporated into battery cells as positive electrodes (cathodes). Thermo gravimetric analysis, infrared spectroscopy, scanning electron microscope and X-ray powder diffraction were used to characterize the silver copper oxides. The materials were tested versus lithium in an electrochemical battery cell. The SCO's were found to have an average capacity of ~ 330 mAh g⁻¹, an average life of 50 hours for complete discharge and an average voltage of 2.2 V.

Using Self-Assembling Monolayers (SAMs) to Improve the Interfacial Strength of a Composite. *LAURIE MOYNIHAN (Washington State University, Pullman, WA 99163) KEVIN SIMMONS (Pacific Northwest National Laboratory, Richland, WA 99352).* Glass fiber materials are used in many aerospace, automotive, and recreational technologies. Oftentimes, the glass component of these

composites is E-glass. Therefore, the strength of E-glass is of paramount importance in the strength of the materials. Shear stress, which most often causes mechanical strain to a glass fiber composite, breaks the bond between the resin matrix and the glass fiber reinforcement. Research was done to determine a new sizing that could be placed on the E-glass fibers to improve the bond between the resin and the glass fibers. The sizing was a self-assembling monolayer. Once the glass fibers were coated with the finish, the glass fiber panels were made with a thermosetting polyester resin using wet lay-up techniques. The panels were placed in a hydraulic press for a minimum of 4 hours to allow for appropriate curing. The glass fiber samples were tested for strength using short beam shear, flexural, and tensile methods. The data collected for the experimental sizings are inconclusive because more testing remains to be conducted. Initial findings do show significant increases over the greige panels and some increases over the commercial sizing. Therefore, new finishes could be developed to use for commercially made glass fiber to increase its strength.

Hydrogen Diffusion in Amorphous Silicon Photovoltaic Solar Cells. *RYAN QUILLER (Rensselaer Polytechnic Institute, Troy, NY 12180) HOWARD BRANZ (National Renewable Energy Laboratory, Golden, CO 89401).*

Hydrogenated amorphous silicon (a-Si:H) is used as a low-cost semiconductor in a range of consumer products because of low production costs. However, they have captured only 10% of the photovoltaic market because of their low efficiencies. This problem is caused in part by hydrogen diffusion, which occurs because a-Si:H is grown at elevated temperatures and because of light-induced degradation. Both problems cause the formation of dangling bond defects. Therefore, in order to better understand hydrogen diffusion in solar cells, a-Si:H i-p-i-n-i structures were made with deuterium tracer layers. These designs were annealed at temperatures similar to their deposition temperatures in order to analyze deuterium diffusion. Secondary ion mass spectrometry (SIMS) data was taken on each sample. A greater dynamic range of the SIMS data was attained than in similar previous experiments by Branz and Nelson since SiD4 was used during deposition of the tracer layer instead of D2. The SIMS concentrations and depths were scaled for consistency. Analysis focused on deuterium release rates. The results of this work support previous findings by Branz and Nelson that hydrogen moves as H⁺, H⁰, or H⁻ depending on the local Fermi level in the a-Si:H device. The activation energy for deuterium emitted from 120 Å from the p- and n-layers were 1.16 eV and 0.81 eV, respectively. These findings illuminate the nature of mobile hydrogen in a-Si:H and could lead to improved photovoltaic efficiencies.

Preparation of Advanced Glasses and Ceramics. *LARA ROGERS (Massachusetts Institute of Technology, Cambridge, MA 02139) S K SUNDARAM (Pacific Northwest National Laboratory, Richland, WA 99352).*

Summer work for the preparation of advanced glasses and ceramics has consisted of three separate tasks. These tasks are briefly summarized below. 1) Suitable high-level waste (HLW) glass compositions with high and low foaming tendencies have been identified, in consultation with a peer and expert in this field. A 1-kilogram sample of each of these compositions has been prepared and sent to the Massachusetts Institute of Technology (MIT) for millimeter wave diagnostic testing. 2) Six samples of two different quantum-droplet producing glasses (sodium borate and borosilicate) have been prepared in the undoped as well as doped forms (with dopants Si and CuO) and characterized, using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The binary undoped compositions have been chosen for their simplicity and phase separation tendency. The dopant is expected to partition with one of the phases that separate in the melt. Samples of these glasses have also been sent to MIT for further characterization. 3) A phosphate-bearing ceramic using samarium as a surrogate for plutonium and americium has been prepared and characterized using x-ray diffraction (XRD), leach testing, and ion chromatography.

Rapid Solidification Process Tooling. *SHAUN SALISBURY (Brigham Young University, Provo, UT 84604) KEVIN MCHUGH (Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID 83415).*

One of the most pressing requirements for manufacturer's of many

processes is the need to reduce tooling delivery time. Rapid Solidification Process Tooling (RSPTM Tooling) can be used to substantially reduce the tooling delivery time. The main objective of RSP Tooling is to produce tooling dies by spraying atomized metal onto a substrate (typically ceramic). H13 Tool Steel (or other alloys) is brought to its liquid state and then heated approximately to 100° C above the melting point. The metal is atomized by a high velocity inert gas stream, which then carries the metal droplets and deposits them onto the substrate where it forms to the shape represented in the pattern. Because of the small size of the droplets (approximately 20 microns), intricate details are attainable. Once the deposit has been sprayed to a desired thickness, the ceramic pattern is removed by grit blasting. The material, as sprayed, was found to have a hardness of 59 HRC. Age hardening can increase this to a peak hardness of 62 HRC. After the aging process, the material is stronger than standard heat-treated H13. In an actual test run of a die casting operation, the RSP insert lasted 25 percent longer than the premium grade H13 insert. The RSP Tooling process shows not only reduced time to produce tooling, but also enhanced properties. It also reduces the amount of energy used to attain the final product. Basically you can get a better tool in a shorter amount of time.

A Non-destructive Technique to Measure the Structural Quality of Cadmium Zinc Telluride. JESSICA SHAWLEY

(Whitworth College, Spokane, WA 99251) MARY BLISS (Pacific Northwest National Laboratory, Richland, WA 99352).

Cadmium Zinc Telluride (CdZnTe) crystals have properties conducive for room temperature radiation detection. Due to the high atomic mass, wide band gap, and good charge carrier mobility, it is a very attractive material. However, lack of understanding of the behavior of trapping levels in the band gap has restricted its advancement as a commercial detector. Such levels are caused by intrinsic defects and impurities, which control carrier mobility and electrical compensation of the material. This paper examines the practice of x-ray diffraction, with a focus on high-resolution x-ray reciprocal space mapping, a form of x-ray diffraction. X-ray reciprocal space mapping has recently been established as a non-destructive and powerful method for strain and structural characterization of epilayers and heterostructures. Continued research on this subject is necessary to help identify which techniques of x-ray diffraction are best suited for non-destructive measurements of the structural quality of CdZnTe. The driving force behind the research is the industrial need for characterization and control of the high-quality crystals that form the heart of so many devices in the science and engineering world. Researchers need to enhance their understanding of the structural quality of CdZnTe without harming the crystal for further study and use as a room-temperature radiation detector.

Friction Stir Surfacing (FSS) of Cast Aluminum Alloys. DANIEL STORJOHANN (South Dakota School of Mines and Technology, Rapid City, SD 57701) STAN DAVID (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Friction stir processing (FSP), a derivative of the rapidly developing friction stir welding (FSW) process, uses frictional heating and plastic deformation to modify the surface of a material. In this process, a rotating pin tool is used to create the frictional heat needed to plastically deform the surface of a component. The microstructural evolution of the plastically deformed surface is expected to increase fatigue, wear, and corrosion resistance. The focus of this research is to modify the surface of aluminum alloys through FSP and to determine its effect on the microstructure and properties. The two common aluminum alloys used in this are A-319 and A-356. Optical microscopy and microhardness testing were used to characterize the shape and size of the stir zone. FSP annihilated porosity and refined the coarse eutectic microstructures associated with cast A-319 and A-356 aluminum alloys.

Development of Friction Stir Welding Pin Tool Design. ADAM WATTERSON (South Dakota School of Mines and Technology, Rapid City, SD 57701) GLENN GRANT (Pacific Northwest National Laboratory, Richland, WA 99352).

Friction Stir Welding (FSW) is a recently developed welding process, patented by TWI Ltd., that is revolutionizing the welding community. It has consistently shown its superior weld quality over typical fusion welds. In addition, FSW has considerably advanced its efficiency and capabilities in order to compete with today's fast paced arc-welding

machines. The tool's design has improved in order to increase the rate of the tool travel speed while maintaining adequate weld consistencies. New geometries have shown promising advancements of the overall process's efficiency. These advancements of the FSW process will lead to more efficient welding applications in the future.

Advanced Nanoporous Composite Aerogels for Industrial Heat Applications. ASHLEY WHITE (Virginia Polytechnic Institute and State University, Blacksburg, VA 24061) ARLON HUNT, MICHAEL AYERS (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Aerogels contain an open pore network of mesopores and a tortuous solid network of nanometer-scaled solid particles making them ideal for use as thermal insulators. One main application of a particularly thermally-resistant aerogel is as an insulator and corrosion resistor in high-temperature furnaces and thermal processing equipment in industrial applications. The objectives of this research were to create a composite aerogel that could withstand temperatures of up to 1000 degrees C and to optimize these gels by maximizing their surface area while minimizing their density. Aerogels were made from CrO₃ and Al(OH)₃ precursors as these substances provide the best thermal insulation for their lowest cost. To optimize the aerogel, several variables were examined, including: the ratio of CrO₃ to Al(OH)₃, the addition of silicon alkoxide precursors, the solvent in which the reaction was performed, and the amount of solvent used. The aerogel's thermal performance was predicted by measuring the surface area and density of the gel, both before and after baking the gels at 1000 degrees C for one hour. In addition, the baking environment was varied in hopes that some atmospheres would promote less aerogel shrinkage during baking than others. The results showed that the optimal ratio of CrO₃ to Al(OH)₃ was 1:2; the addition of silicon alkoxide precursors increased the surface area and decreased the sintering of the gels, with TEOS performing the best; ethanol was the best solvent; a large amount of solvent gave the least dense gels; and the type of atmosphere in which the gels were baked had negligible effect on their density.

The Synthesis of Molecular Based Precursors for the Construction of Molecular Superconductors, Magnets, and Hybrid Materials. MICHAEL WHITED (Lewis University, Romeoville, IL 60446) JOHN A. SCHLUETER (Argonne National Laboratory, Argonne, IL 60439).

The first purely organic superconductor [b'-(ET)₂ SF₆CH₂CF₂S₀] was synthesized with the electrocrystallization technique by a team of chemists in 1996 at Argonne National Laboratories. Since that time or shortly after, efforts have shifted from heavily fluorinated organosulfonate anions to dicyanamide complexes. The search for superconductors, molecular magnets and/or hybrid materials using [N(CN)₂] ligands with metals such as, (M= Mn, Co, Ni, Cr and Cu) is the primary goal and focus. The ideal is to incorporate the magnetic dicyanamide anion layer into conducting charge transfer salts; thus coupling conductivity with magnetism. The synthesis of new molecular based precursors for the construction of molecular superconductors, magnets and hybrid materials includes synthesis of highly conductive/ superconductive and/or magnetic charge transfers. I have learned about synthesizing and characterizing molecular based precursors for superconductivity, magnetism and hybrid materials and how to potentially synthesize these materials from electrocrystallization process. My main goal is to synthesize molecular based precursors that will crystallize with the ET molecule to produce organic superconductors and/or conducting/magnetic hybrids. It is hopeful that new materials will provide a couple affect between the conducting and magnetic sublattices and lead to application in devices.

Ruthenium Partitioning in a High-Level Waste Glass. TAMMY WILLWATER (Pima Community College, Tucson, AZ 85730) S.K. SUNDARAM (Pacific Northwest National Laboratory, Richland, WA 99352).

Vitrification, a process that stabilizes hazardous/nuclear waste by incorporating them into a glass, is a practical solution to the disposal of nuclear waste from the beginning of the nuclear era. Once crystals are formed in glass melt, they tend to settle down in a melter, which could potentially lead to power fluctuations, current excursions, and even shorting of electrodes causing melter failure. It is important to understand the solubility of noble metals as well as their partitioning between the crystal phase formed and the glass. Research will continue on this particular subject for many years to come. This

investigation studied the partitioning of ruthenium in a model high-level waste glass (MS-7). Ruthenium oxide was used because it is predominantly found in melter tests with feeds containing noble metals at the bottom of the melter. Ruthenium oxide concentrations of 0.1 %, 1 %, and 10 % were used in doping the glass to saturate the melt above its limited solubility. This simulates somewhat the conditions in the bottom of the melter where noble metals accumulate. The heat-treatment conditions (temperature and duration) were chosen from reported literature (Alton et al. 2001), such that large crystals of trevorite (NiFe₂O₄) were formed in the glass. Samples were prepared for scanning electron microscopy (SEM) and microprobe characterization. SEM results showed the crystals distributed in the glass matrix. Microprobe measured the ruthenium concentration across the glass-crystal interface. The results are summarized in this paper.

Synthesis and Characterization of Spatially Confined Metal Nanoparticles. AMANDA WOLF (University of Illinois, Urbana-Champaign, IL 61801) MILLICENT FIRESTONE (Argonne National Laboratory, Argonne, IL 60439).

Metal nanoparticles are prepared in situ within a lipid-based complex fluid. Complex fluids have the unique ability to spontaneously self-assemble into an organized lattice of layers based upon the chemical properties of its components. Current research involves continuing the study of polymer-grafted, lipid-based complex fluids that are composed of aqueous metal salt precursor solutions, a phospholipid, terminally grafted with a hydrophilic polymer head group, and a phospholipid. Prior studies have demonstrated that these specifically designed complex fluids can be used to spatially organize inorganic nanoparticles based on their size and surface chemistry. The effect of spatial confinement on the optical properties of the nanoparticles was also assessed. Unlike previous research, where nanoparticles were created prior to being introduced to a complex fluid, the research described herein examines the in situ synthesis of metal nanoparticles. This work expands the range of the synthetic techniques by which the nanoparticles can be prepared and their physical properties tuned. This work represents an important first step toward the use of nanoparticles and structures to create smaller, more powerful "nanoscale" machinery, such as computers and other electronics, which is of such particular interest to many fields of study at this time.

MEDICAL AND HEALTH SCIENCES

bFGF as a Radioprotectant in Two Animal Models. KATHERINE AUDETTE (St. Olaf College, Northfield, MN 55057) LOUIS PENA (Brookhaven National Laboratory, Upton, NY 11973).

Advancements in cancer treatments are dependent upon a better understanding of both normal and abnormal cell growth paired with an extensive exploration of potential treatment venues. Modulating the radiation tolerance of normal cells might enhance the effectiveness of radiation therapy. Certain synthetic cytokines that have been developed as analogs to basic Fibroblast Growth Factor are being analyzed to determine their protective effects against apoptosis. Mice were total body irradiated to induce gastrointestinal syndrome after retro-orbital or gavage administration of bFGF. Mice treated with the growth factor survived longer compared to controls. To test the effectiveness of bFGF in localized radiation damage to the salivary glands, rats were locally irradiated at the parotid gland region and 1 and 5 days later glands were harvested and stained for apoptosis. Samples were evaluated qualitatively and determined to have a reduced incidence of apoptosis in the presence of bFGF. These results support previous studies that found FGFs to possess radioprotective qualities. The development of a synthetic version of bFGF will be advantageous as it can be manufactured as needed and carefully controlled for quality. These substances may be incorporated into radiation cancer treatment for their selectivity and cell protecting qualities.

Examining Differences in Dopamine Receptors Between P and NP Rats by Autoradiography. ANDREW BOOHER (Bradley University, Peoria, IL 61606) PANAYOTIS K. THANOS (Brookhaven National Laboratory, Upton, NY 11973).

The role of the dopamine neurotransmitter in various addictive behaviors, including alcohol abuse, has been well documented. In an attempt to generate a rodent model of alcohol abuse, the Indiana Alcohol Research Center has developed alcohol preferring (P) and non-preferring (NP) rats. This study used autoradiography, a common

method for both qualitatively and quantitatively imaging animal brains, to study the differences in dopamine receptor levels between these two strains. Autoradiography was performed on both P and NP rats. Each animal's brain was removed, sectioned, and labeled with [3H] raclopride, a ligand that binds to the D2 dopamine receptor. These sections were then examined by a PhosphorImager to determine the intensity of the raclopride in different structures of the brain. Ultimately, the NP rats had significantly greater binding than the P rats in the striatal region (13.81 ±0.47 vs. 11.46±0.72, P=0.007) and a greater binding ratio of striatum to background (10.66±0.42 vs. 8.97±0.57, P=0.018). These results add support to the conclusion that individuals with lower levels of dopamine receptors are more likely to engage addictive behaviors.

Dose Tolerance Factors in Microbeam Radiation Therapy. REBECCA CURRELL (Washington State University, Pullman, WA 99163) AVRAHAM DILMANIAN (Brookhaven National Laboratory, Upton, NY 11973).

There are over 8,000 cases of high-grade gliomas in the United States a year. Although current treatment of these tumors has strong palliation effects, they do not produce any definitive cures. Conventional radiotherapy (XRT) also cannot be used on children under the age of three because of their more radiosensitive brain tissue. Current research with animals, on a type of spatially fractionated radiation (SFR) therapy called microbeam radiation therapy (MRT), may be a better solution to these problems.

Inhibition of Acetylcholine Release in Brain Slices by Endogenous Anandamide. CAMILE GOODEN (State University of New York at Stony Brook, Stony Brook, NY 11790) ANDREW GIFFORD (Brookhaven National Laboratory, Upton, NY 11973).

It was observed in previous studies that exogenous cannabinoid receptor agonists have an inhibiting effect on the electrically stimulated release of acetylcholine (ACh) from superfused brain slices of the hippocampus of rodents (Gifford, Ashby 1996). The mechanism proposed for this inhibition involves the binding of specific ligands to CB1 cannabinoid receptors located in abundance in the hippocampus. One such ligand is the natural brain lipid known as anandamide. This study is aimed at observing the effect that endogenous anandamide has on the release of acetylcholine in rat hippocampal brain slices. The endocannabinoid anandamide is released in the brain by pyramidal cells when they become depolarized. Depolarization of these cells can be achieved by the binding of metabotropic glutamate agonists on the metabotropic glutamate receptors located on the pyramidal cells. Metabotropic Glutamate agonist drugs such as DHPG, ACPD, DCGIV and Picrotoxin are used in various concentrations and combinations to help increase the potency and concentration of endogenous anandamide and exponentiate its effect on stimulated acetylcholine release in hippocampal brain slices. In the present study it was discovered that there is indeed an inhibition of acetylcholine release when metabotropic glutamate agonist drugs are added to the superfusion medium of hippocampal brain slices prior to stimulation. Future experiments will be to determine if this inhibition is mediated via anandamide release in the brain slices by examining the effect of cannabinoid receptor antagonists on the glutamate agonist mediated inhibition of acetylcholine release.

Promotion of Wound Healing by bFGF. BRYAN GRACKIN (The George Washington University, Washington, DC 20052) LOUIS PENA (Brookhaven National Laboratory, Upton, NY 11973).

The process of tissue repair consists of a sequence of events including infiltration of specialized cells to the injury site. The platelets and inflammatory cells are the first cells to arrive and they provide key functions for the creation of connective tissue cells and new blood. These cells are known as growth factors or cytokines. In this experiment, Adult Fischer 344 rats (female) were used. Bilateral full thickness wounds were made on the back behind the shoulders. Fur was shaved and two points 10 mm apart were marked on the skin. Skin between those points were grasped with calipers and cut with fine-tipped straight scissors to affect a full thickness wound of ~ 10x12x3 mm. A drop of sterile saline was placed in the wound space and a thin polyurethane film placed over it. The film was either uncoated or coated with bFGF. Animals were sacrificed at day ten during the height of cell proliferation. Adhesive bandages were placed

over the thorax of the animals to protect the wound. The bandages were removed and tissue of the wound area or controls were surgically removed, fixed in formalin, and embedded in paraffin and processed for histological analysis. It was found that bFGF coated bandages caused increased fibroblast proliferation compared to control.

The Effect of Nicotine and Δ^9 -Tetrahydrocannabinol on Dopamine Neurons in the Ventral Tegmental Area and Substantia Nigra in Rats. TANGERINE HALL (*Monroe Community College, Rochester, NY 14623*) ONARAE RICE (*Brookhaven National Laboratory, Upton, NY 11973*).

With the administration of some common addictive drugs, such as nicotine and Δ^9 -Tetrahydrocannabinol (Δ^9 -THC) the concentration of extracellular dopamine has been shown to increase within the nucleus accumbens (NAcc). As the major psychoactive ingredient in marijuana, studies on Δ^9 -THC suggest that it facilitate dopamine neurotransmission and that this effect plays a major role in the reinforcing property of the drug. Nicotine, the major component of tobacco has also been proven to continually stimulate dopamine release. In the present study single cell electrophysiology recording was used to monitor the activity of nicotine and Δ^9 -THC on dopamine neuron firing rates within the substantia nigra (SNc) and ventral tegmental area (VTA). These studies were conducted in anesthetized male Sprague-Dawley albino rats (150-300g). Neuronal firing was monitored on an oscilloscope and presumptive dopamine neurons are identified after meeting certain criteria. With the classification of a dopamine neuron, intravenous injections of nicotine and/or Δ^9 -THC were given. In previous studies it has been documented that intravenous administration of nicotine and Δ^9 -THC stimulate a dose-related increase in the firing rate of A9; (originating in SNc) and A10; (originating in the VTA) dopamine neurons. However in our current study of the SNc and VTA brain regions we were not able to confirm the effect(s) of these drugs on dopamine neuronal firing rate in either the SNc or VTA.

Effects of Drugs of Abuse on Brain Dopamine: [3H]-Raclopride and Dopamine Competition in Mouse Striatal Tissue in vivo. NAQI KHAN (*Cornell University, Ithaca, NY 14853*) S. JOHN GATLEY (*Brookhaven National Laboratory, Upton, NY 11973*).

Dopamine is a neurotransmitter that is vital in regulating motor skills and judgment, while also influencing substance abuse and addiction. This study concerns the release of dopamine and its binding to dopamine receptors, localized in regions of striatal tissue within the brain of a mouse. Dopamine release was stimulated through the injection of drugs such as nicotine and tetrahydrocannabinol (THC) into the mice subcutaneously (s.c.) and intraperitoneally (i.p.). To gather a quantitative measure of the binding of dopamine, a radioligand, [3H]-raclopride (RAC), was also administered into the mouse. RAC binds to dopamine receptors and is expected to compete with internally released dopamine. The amount of RAC in the striatal tissue can be detected utilizing a scintillation counter. The RAC present in the striatal tissue is believed to be a direct measure of dopamine concentration in the synapse (the space between the nerve cells). A greater amount of RAC implies a lower concentration of dopamine, whereas a lower amount of RAC indicates a higher concentration of dopamine. The results showed considerable variability, however, and raised the question of whether the novel experimental conditions (to the mice) affected the levels of dopamine. However, a slight trend in the data suggests increased competition between RAC and dopamine in mice injected with nicotine or THC. A better experimental paradigm was designed for extending this work.

An Introduction to Function and Origin of Oligodendrocytes; Microbeam Radiation Therapy Effects on Oligodendrocytes. JESSICA KRAMER (*Sinclair Community College, Dayton, OH 45402*) AVRAHAM DILMANIAN (*Brookhaven National Laboratory, Upton, NY 11973*).

Conventional radiation therapy (XRT), which is a main method of treating brain tumors, could cause irreversible damage to the surrounding central nervous system (CNS) tissue. The main late effects of XRT, namely demyelination of the brain, is caused by the XRT damage to oligodendroglial cells. An innovative type of radiation therapy, microbeam radiation therapy (MRT), is thought to minimize damage to the normal tissue in general, and oligodendroglial cells in particular. The experiment presented here uses arrays of x-ray microbeams to irradiate normal rat brains and rats with implanted

tumors to study the biological mechanism behind MRT's sparing of the normal brain and preferential tumor killing. The rats are kept for certain time points, then euthanized either by tissue perfusion or another way to enable extraction of the brain for histological analysis. The current experiment is still in progress and no final results of the therapeutic effects have been examined. This research discusses the potential effects of MRT on oligodendrocytes, and describes the experiment that was carried out to study MRT's biological effects.

The C57Bl/6 Mouse as a Behavioral Model to Assess Drug or Space Radiation Induced Toxicity to the Central Nervous System. JENNIFER OTT (*Suffolk County Community College, Selden, NY 11784*) MARCELO VAZQUEZ (*Brookhaven National Laboratory, Upton, NY 11973*).

The drug methamphetamine, a psychostimulant used widely as a recreational substance, can lead to neurotoxicity when taken at high doses. The neurotoxicity is a result of dopamine release in the synapse leading to the promotion of free radicals causing oxidative stress. An acute toxic treatment of methamphetamine in 10 mg/Kg and 15 mg/Kg doses were given to C57Bl/6 mice. This same strain was used for the control group, which was given saline. The mice were placed in photocell boxes which were used to test locomotor activity for a one hour period 1, 3, 7, and 14 days after treatment. The locomotor activity of the methamphetamine treated mice decreased 24 hours after treatment. Three days after animal injections, the results showed an increase in the locomotor activity and a continued increase at 7 and 14 days. These observations can be explained through a possible compensation mechanism, which may have occurred in an attempt to recover from oxidative stress. We propose that a longer period of treatment, different from current acute toxic dosing models, may be necessary to create more sustained and measurable behavioral changes in C57Bl/6 mice after MA treatment.

Apoptosis in a Brain Tumor Model. CHRISTINA RAGER (*State University of New York at Stony Brook, Stony Brook, NY 11794*) LOUIS A. PENA (*Brookhaven National Laboratory, Upton, NY 11973*).

Even with the advanced cancer treatment methods that have been developed and tested over time, malignant brain tumors remain one of the most difficult and dangerous types to treat. Thus, it has become increasingly important to increase the efficiency of non-invasive therapeutic methods. Radiation therapy is one of the most promising techniques due to its ability to trigger cellular apoptosis, or programmed cell suicide. If it were possible to increase the sensitivity of malignant cells to radiation, they may be more easily eliminated while surrounding tissue may be protected and less affected. It seems reasonable to believe that by modifying the apoptotic signaling pathway, such sensitization may indeed be possible. This research involves the investigation of ceramide, a lipid molecule that may act as a second messenger in the SAPK/JNK signaling pathway, and how up- and down-regulation of distinct enzymes of ceramide metabolism affect cellular levels of apoptosis. While its role in the apoptotic pathway has become a heavily disputed topic, these results indicate that the presence of ceramide may actually suppress the apoptotic response. The other main focus of this project is to perform a generalized dissection of the caspase signaling cascade, which has also been under much scientific scrutiny. The final goal is to uncover how radiation-induced apoptosis signals may be transduced via ceramide and the caspases in a brain tumor model.

Analysis of In Vivo Measurements Results of 40K in Hanford Workers. JAMES RIVARD (*Yakima Valley Community College, Yakima, WA 98907*) TIM LYNCH (*Pacific Northwest National Laboratory, Richland, WA 99352*).

A population of female and male employees at the US Department of Energy's Hanford site near Richland, Washington has been monitored at the In Vivo Radioassay and Research Facility (IVRRF) over the past forty years for whole body content of 40K. The measurement of radionuclides has been conducted using gamma-ray spectrometry using a variety of counters: including NaI detectors in chair, shadow shield, and standup geometries as well as coaxial germanium detectors in a supine geometry. Various nuclides have been detected and recorded using the whole body counters, but this particular study focuses on the naturally-occurring radionuclide 40K. Results from the years 1960, 1970, 1980, 1990, and 2000 were studied. The Hanford workers were separated based upon gender. Gender categories were then subcategorized into total body potassium (TBK), nCi activity

level, and grams potassium per kilogram. The categories were further evaluated as a function of age, weight, and body mass index (BMI). Males tended to have higher concentrations of potassium than females, due to a larger muscle vs. fat tissue ratio (Kathren, 1984). Males had $23\% \pm 10\%$ higher average TBK, when compared to females within the same year. Potassium concentration and TBK decreased with age. Potassium concentrations also decreased with increasing BMI, and BMI increased with age, which suggest that most weight gain in elder years is fat tissue with lower potassium concentrations. Future analysis of 40K and potassium concentrations should include studies of single individuals over an extended period of time, and a perspective on slenderness index.

The Chronic Effects of Oral Methylphenidate on Dopamine Receptors: An Autoradiographical Assessment. *SETH RIVERA (Syracuse University, Syracuse, NY 13244) PANAYOTIS THANOS (Brookhaven National Laboratory, Upton, NY 11973).*

Attention Deficit Disorder is a widespread neuropsychiatric condition that affects approximately 5% of the U.S. population of school-aged children. The oldest and most commonly used stimulant medication is methylphenidate. Over 1.5 million children between the ages of five to eighteen were taking methylphenidate in 1995. This is a medication that some children take for years. Despite widespread use of this medication for over fifty years, little is known about its long-term physiological effects. The purpose of this study is to examine striatal dopamine (D2) receptor availability in non-drug treated subjects as compared to those receiving methylphenidate treatment using autoradiography. The dopamine receptor downregulation has been hypothesized to underlie the reward deficiency syndrome, a state of chronic anhedonia relieved only by actions that increase intrasynaptic dopamine: drug use or novelty seeking. Previous studies using PET imaging indicate that subjects treated with methylphenidate show decreased D2 binding in the striatum, supporting the hypothesis that ADHD individuals undergoing drug therapy are at greater risk for drug abuse in later life.

Proactive Reduction of Injuries at Work through Ergonomics Methods. *JEANNETTE SANTOS (University of Puerto Rico, Cayey, PR 00736) PATTI BENDER (Brookhaven National Laboratory, Upton, NY 11973).*

In order to reduce occupational injuries, Environmental, Safety & Health Professionals from Brookhaven National Laboratory performed a research project to reduce injuries by proactively involving workers in injury prevention training activities. This initiative had three different phases. After creating focus groups from the three highest injury groups on site (custodians, electricians, and site maintenance), each focus group had meetings to identify work task risks and prioritize them for further subject matter expert ergonomic analysis. Focus group members and custodians used the Washington Ergonomics Task Evaluation Booklets as the evaluative tool as the student's awareness of extreme and neutral position to prevent injury is crucial to their safe work performance. The evaluation data collected from the custodians in 1998 showed that by identifying and assessing risks in the workplace and then training workers to be aware of extreme and neutral positions and postures to perform their tasks; it is possible to reduce the potential for certain types of occupational injuries. This data was summarized and conclusions drawn as presented in this research paper. BNL staff working with this new data will analyze and recommend task improvements to proactively address these risks thereby minimizing the potential for future injuries.

Microbeam Radiation Therapy in Relation to Endothelial Cells and Thrombosis. *MONICA SAWICKI (Housatonic Community Technical College, Bridgeport, CT 06614) AVRAHAM DILMANIAN (Brookhaven National Laboratory, Upton, NY 11973).*

Conventional radiation therapy (XRT) currently used for the treatment of brain tumors is not curative for certain types of highly malignant tumors. This is because the dose necessary to control the tumor can also damage the normal brain around it. The brain damage is mediated partly by endothelial cells (EC). An experimental type of radiation therapy called microbeam radiation therapy (MRT) is being used to determine its effects on the rat's central nervous system and brain tumors. MRT differs from XRT because it uses spacing within the beam to allow for a peak and valley dose to hit the area treated in the brain. The peak dose is the amount of radiation used to treat the tumor. The valley dose within the spacing is less than the substantial dose

used for treatment, allowing normal cells as well as tumor cells within it to survive. Previous experiments based on this type of radiation show that it is less damaging to normal tissues based on the hypothesis that the certain types of cells such as ECs within the valley dose can regenerate and replace damaged cells. Yet, this repair mechanism somehow fails in the tumor's vasculature. Thrombus can also occur within the peak dose in the tumor's capillaries, cutting the blood supply and causing the tumor to starve to death. In order to perform this experiment, fifty rats were used. All rats were euthanized at different time points by tissue perfusion to allow for an investigation through microscopy as to how their brains were affected. Some rats had to be taken out before their actual time points because they were showing symptoms related to death by tumor growth.

The Role of Dopamine D2 Receptors (DRD2) in Obesity: A Rodent Model. *BRITTNEY TEJADA (Southern Utah University, Cedar City, UT 84720) GENE-JACK WANG (Brookhaven National Laboratory, Upton, NY 11973).*

ABSTRACT The mechanism(s) underlying obesity or overeating is not well understood. The dopamine neurotransmitter is among the possible factors that are involved. Here we used Zucker rats, which have a leptin deficiency that make them more prone to becoming obese. There are two types of Zucker rats: lean (Le) and obese (Ob). The present study consisted of 4 groups: 1) Obese (Ob)- previously unrestricted diet (PUD), 2) Ob - previously restricted (20 g/day) diet (PRD), 3) Lean (Le)- PUD, 4) Le - PRD. Data was collected from 25 - 32 weeks and consisted of the following: 1) Body weight - which showed that Ob-UD had a significantly greater body weight than the Le-UD ($p < 0.001$), Le rats were significantly more active. Apomorphine test at 30 weeks showed no significant difference between groups ($p=0.117$). Test done at 32 weeks showed a significant difference between groups when injected with saline.

NUCLEAR SCIENCE

Automation of Quantitative Microscopic Methods for the Purpose of Determining Phase Ratios in Irradiated Research Reactor Fuel. *RICHARD BRAZENER (Juniata College, Huntingdon, PA 16652) MITCHELL K. MEYER (Argonne National Laboratory, Argonne, IL 60439).*

Quantitative microscopy is a statistical process that can determine volume ratios of phases in the internal structure of metals by overlaying a grid and classifying points. Previous methods of determination consisted of manually applying the grid and tabulating results. The purpose of this research was to develop an automated process that could accomplish this task with the same degree of accuracy as the original methods. The automating of this process was accomplished by writing a custom point counting program in the Java programming language. The results of determinations of ratios of different phases from micrographs with uranium-molybdenum research reactor fuels using the program were compared to previous results. The results were in agreement by within 5%, indicating similar accuracy between the methods. Further automation can be implemented for the measurement of other parameters, such as interaction layer thickness between the fuel and matrix phases.

Quantitative and Qualitative Analysis of Distillate Fuel Performance. *GREGORY CACACE (Suffolk County Community College, Selden, NY 11736) WAI-LIN LITZKE (Brookhaven National Laboratory, Upton, NY 11973).*

This effort is the first in-depth field study on burner fuels that will provide answers on the magnitude and impact of fuel quality on residential heating system performance. Poor fuel quality causes a heating system to fail in performing its design function. The ultimate aim is to eliminate fuel quality related service calls, and to develop analytical tools to help the industry with a major fuel problem. It is important to realize that over an extended period of time fuel oil will degrade through oxidation and condensation in the tank. Poor maintenance at storage facilities can lead to water and sludge buildup from particulates and microbial growth. The laboratory studies will be designed to analyze specific fuel properties in controlled settings. ASTM (American Society for Testing and Materials) standards for analyses will be used where applicable so that data generated could be compared. These tests will address issues related to how quickly fuel oils age, how long they can be stored before they become

unacceptable, how sulfur content impacts stability, and the effects of soluble metals in the heating system. The field studies, are being conducted to look at fuel characteristics from the source and along the distribution chain, down to the end-user tanks. The analyses will consist of quantitative and qualitative properties generally considered minimum requirements for distillate product acceptance. The laboratory studies will also include additional analyses that are relevant to the specific fuel properties being studied such as sulfur content, stability by oxygen overpressure, contact with copper and corrosion factors, and bottom sediment and water analysis.

Precision Measurement of Branching Ratios in Na-21 Beta Decay. AIDAN CRAIG (*University of California - Berkeley, Berkeley, CA 94704*) STUART FREEDMAN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Our research effort seeks to determine ^{21}Na 's beta-branching ratio to the 351 keV excited state. Efforts will be made to improve the compilation figure of $5.03 \pm 0.13\%$ (H.S. Wilson et al, Phys. Rev. C, 22, 1696 (1980)) to roughly 0.05% absolute accuracy, which will reduce a sizable source of systematic uncertainty in measurements of other properties of ^{21}Na decay with the Facility for Exotic Atom Trapping at the LBL 88" Cyclotron. The ^{21}Na source will be generated from a 14 MeV proton beam via the ^{21}Na decay with the Facility for Exotic Atom Trapping at the LBL 88" Cyclotron. The ^{21}Na source will be generated from a 14 MeV proton beam via the $^{24}\text{Mg}(p,\alpha)$ reaction. High-resolution spectroscopy will then be performed with a pair of approx. 300 cm³ HPGe detectors borrowed from the GAMMASPHERE experiment. The branching ratio will be found from the height of the 350+511 keV sum peak, which unlike the 350 keV peak is uncontaminated by the 511 keV peak's 340 keV Compton edge. The measurement's accuracy is affected by uncertainties due to statistical variation and the accuracy of the detectors' efficiency calibration at 350 keV. A high-precision 350 keV calibration will be made by analysis of ^{21}F 's 1395-351 keV gamma-ray cascade, and supplemented with a second, off line measurement of the 356-81 keV cascade of a ^{133}Ba sealed source. At present, online data collection is scheduled to begin no earlier than October, but this summer's preliminary studies of the physics and equipment involved in the experiment have not uncovered any insurmountable obstacles to our stated goal of 0.05% absolute accuracy.

Recent Progress in Beam Diagnostics for Heavy Ion Fusion. CHARLES DUGAN (*Rensselaer Polytechnic Institute, Troy, NY 12180*) FRANK BIENIOSEK (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Beam characterization is important in the development of a heavy ion driver for inertial confinement fusion. A method of using the polymer kapton as a film has been implemented to create relative beam intensity data, and various image-processing issues involved with this method are addressed. Investigation into the use of a sintered alumina wafer as a scintillator to image the beam is discussed, and an experiment to determine the specific photoemission sensitivity of alumina to ions and electrons has been performed. After calibration of the photomultiplier tube, and correction for other effects such as the optical transmission of the alumina wafer, the quantum efficiency of the scintillator was measured as a function of the energy of the incident particles. Electrons often complicate beam diagnostics, so it is important to be aware of their effect on the diagnostic. Therefore, an additional development involved empirically based predictions that also used the Trim2000 Monte Carlo code, which were implemented to create a relationship between ion beam energy and secondary electron yield for K^+ and Cs^+ beams with energies of 10 keV to 30 MeV on various materials.

Modeling of the External Beamline Optics into the Gammasphere at the 88-Inch Cyclotron. GUSTAVO GONZALEZ (*Santa Monica College, Santa Monica, CA 90405*) DANIELA LEITNER (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The 88-inch Cyclotron is currently home to the Gammasphere, the world's most powerful gamma ray detector that has been operating as a national facility since April of 1993. Gammasphere was built to study the complex structure and behavior of nuclei by fusing lighter nuclei into heavier ones and observing gamma rays - a form of extremely high-energy light - emitted when the new nuclei's component protons and neutrons settle into stable configurations. In order to meet the

needs of some of the Gammasphere experiments, a new beamline was constructed with improved vacuum, beam diagnostics, and optics systems. The ion beam transport project is meant to model the beam line running from the cyclotron vault to cave 4C, where the Gammasphere is housed. It is important to model the beam line because different experiments require different parameters. The Gammasphere requires that the beam be about 3mm in diameter when it hits the target. The modeling of the beamline is done using TRACE-3D software.

Analysis of the Low-Energy Background in the Sudbury Neutrino Observatory. SILJA HAAPANEN (*Santa Monica College, Santa Monica, CA 90405*) KEVIN LESKO (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The Sudbury Neutrino Observatory (SNO) is a particle detector constructed for the study of neutrinos coming from the nuclear fusion reactions in the Sun; specifically, for testing the Standard Solar Model (SSM) and solving the solar neutrino deficit problem. The solar neutrino deficit problem resulted from the fact that the number of neutrinos predicted by the SSM differed from the number observed by experiments. The experiments prior to SNO, however, had only been sensitive to one of the existing three flavors of neutrinos, the electron flavor. SNO is sensitive to all three flavors and has solved the solar neutrino deficit problem by providing evidence for neutrino flavor transformations; a neutrino oscillates between different flavor states — electron, muon, and tau -- in transit from the Sun. Neutrinos are very weakly interacting and detecting them is difficult. The detector has to be kept clean from any contamination from radioactivity normally found in the environment; decay of radioactive elements in the detector could result in signals resembling a neutrino event. Analysis for separating low-energy events from the intrinsic background present in the detector therefore becomes an important part of the process. This study concentrated on the time variations of the low-energy background, and the effect of detector operations on the level of radioactivity. The detector operations, such as D2O circulation through its purification system, were not found to have an effect on the rate of low-energy events. However, a time variation in the detector response was observed.

Electron Proton Elastic Scattering. KHAM HO (*Gainesville College, Gainesville, GA 30543*) MARK JONES (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

Measurements of the nucleon form factors provide an important test of the nucleon model. The Rosenbluth technique, which keeps the four-momentum transfer constant and only varies the beam energy and the angle, was used to separate the proton electric and magnetic form factors. Measurement of the proton ratio of the transverse and longitudinal components is an alternative method of measuring the proton electromagnetic form factors. Before the proton form factors can be measured, elastic events need to be identified. In elastic scattering, the electron will be detected by the lead-glass calorimeter, and the proton's total momentum and energy will be measured using the High Momentum Spectrometer (HMS) in Hall C. Elastic events need to be separate from random coincidences and other reactions. A Monte Carlo was written to explore the capabilities needed in the detector to have a clean separation of elastic events.

Using Percolation to Study Surface Effects in Clusterization. SEPEHR HOJJATI (*Contra Costa College, San Pablo, CA 94806*) JAMES B. ELLIOTT (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The multifragmentation data of the ISIS Collaboration was found to follow the scaling of Fisher's droplet model. Fisher's model gives the concentration of clusters (e.g., nuclear fragments) as a function of cluster size and the temperature of the system. The model is based on an estimate of the partition function of a cluster that has both energetic and entropic contributions. While the energetic term is very well understood thermodynamically, the origins of the entropic factor are less understood. Fisher theorizes the entropic factor to have a particular functional form based on the combinatorics of clusters. One way to gain insight into this part of the Fisher's model is to divide the experimental fragment yields by the energetic factor, isolating the entropic portion. For clusters on a two dimensional lattice, we can then compare the result against well-known enumerations of the combinatorics, e.g., that of the self-avoiding polygons (SAPs). In this study we

attempt to examine Fisher's functional form of the entropic factor by using a standard $d = 2$ site percolation on a square lattice. We will first divide the fragment yields obtained from our model by the percolation energetic factor and then compare our result to that of the actual enumerations of the SAPs.

Spectrophotometric Detection of Plutonium using a 1.0-meter Liquid Core Waveguide. YUNG-JIN HU (*University of California Berkeley, Berkeley, CA 94720*) HEINO NITSCHKE (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Detection and quantification of trace metals, in particular actinides, can be achieved through various analytical methods such as mass spectroscopy and radioactive counting. However, these methods used by themselves lack the specificity to identify oxidation state and speciation of actinides in the environment. UV-Vis-NIR absorption spectrophotometry can detect and quantify oxidation states of aqueous actinide ions. Enhancements in detection for absorption spectrophotometry can be made by either complexing the actinide ion with a high-extinction-coefficient organic ligand or increasing the path length of the spectroscopic cell. Since the Beer-Lambert law ($A=εcl$) is directly proportional to both of these factors, changing either or both will increase the detection limit for the system. A 1.0-meter liquid core waveguide was used in this study which included sampling both plutonium aqua ions, in its various oxidation states, and the plutonium-chlorophosphonazo-III complex. The Beer's Law plots of the various plutonium aqua ions showed excellent linearity at low concentrations and the liquid core waveguide produced an increase in limit of detection by 18 to 33 times the calculated limits of detection for a conventional 1.0 cm spectrophotometric cell. Although initial experiments of the plutonium-chlorophosphonazo-III complex show promise as a further method of decreasing plutonium limit of detection for spectrophotometric detection, more experiments are needed before any conclusive statements can be made.

Strong Color Field Effects on Phi-Meson Production in

Relativistic Nucleus-Nucleus Collisions. SRIKUMAR KESAVAN (*Yale University, New Haven, CT 06520*) SVEN SOFF AND NU XU (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

We focus on the production of the ϕ -meson in Au+Au ($\sqrt{s_{NN}}=200$ GeV) collisions at the Relativistic Heavy Ion Collider. The extremely large energy densities produced in such collisions allow for the investigation of new forms of matter, such as the quark-gluon plasma, and their properties. A very interesting feature of relativistically colliding heavy nuclei may be the production of strong color electric fields. In the framework of a relativistic transport model (Ultrarelativistic Quantum Molecular Dynamics), we study these effects by altering two parameters - associated with the strength of the color field and the transverse momentum - on important observables such as mean transverse momenta and particle yields. The importance of the coalescence mechanism of kaons for the production of the ϕ -meson is also studied. Increasing the strength of the color field dramatically increases the production yield of ϕ -mesons. Increasing the transverse momentum broadening parameter decreases the yield of ϕ -mesons, particularly the contribution from the coalescence channel. Both parameters also play important roles in determining the transverse momentum distributions of the particles studied. Increasing the transverse momentum broadening parameter significantly increases the contribution from the string processes to the transverse momentum distribution of the ϕ -meson. The systematics of the mean transverse momentum for various particles are also presented. Moreover, we address the effects of rescattering of the decay products of ϕ -mesons. The analysis is integrated with results from p+p collisions in order to better understand string processes in the production of the ϕ -meson.

Radiation Exposure Pathways from Building 3525. BART LYNCH (*University of Tennessee, Knoxville, TN 37916*) MICHAEL MUHLHEIM (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The U.S. Department of Energy and the U.S. Nuclear Regulatory Commission provide guidance for identifying process and operational hazards to workers and to the public for different hazard types (e.g., radiological, toxic, carcinogen). This study focuses on the potential radiological hazards and the associated radiological consequences from the release of radionuclides at a hot cell facility. Accident analyses typically focus on the activity of the radiological sources (i.e., curies) to calculate direct exposure doses. However, the probability of a member of the public being involved in a direct exposure accident is

very small. Furthermore, as a result of short exposures times and large distances from the source, the consequences associated with such an exposure are also small. The potential inhalation dose from the atmospheric dispersion of radioactive particulate matter has much higher consequences, and thus building limits should be set based on the committed effective dose equivalent (CEDE). Based on initial nuclide inventories of the High Flux Isotope Reactor (HFIR) core at end-of-life, it is possible to predict both the direct exposure doses to personnel in the vicinity of an accident as well as the 50-year CEDE to individuals offsite. OrigenArp was used to simulate a 360-day core cool down. An analysis with selected nuclides indicates that the inhalation dose increases over time. However, when the whole core is simulated, the inhalation dose decreases after cool down, but by a smaller percentage than the direct exposure dose.

Investigation of Optimal Container Specifications for Obtaining Ceramic Waste Form Model Calibration Data. MICHAEL STAWICKI (*Massachusetts Institute of Technology, Cambridge, MA 02139*) KENNETH J. BATEMAN (*Argonne National Laboratory, Argonne, IL 60439*).

When the Experimental Breeder Reactor Number 2 was decommissioned in September of 1994, a method was needed to prepare its highly volatile sodium-bonded spent nuclear fuel for disposal. It was determined that the fuel would undergo electrometallurgical preparation in an electro refiner and that the waste salts would be encased in a solid zeolite ceramic waste form (CWF). To assist in the production of large scale CWFs of several hundred kilograms, a computer model was developed to predict consolidation levels over time at specified temperatures. In order for the model to accurately predict the kinetics of the CWF, thermophysical calibration quantities must be entered for the specific lots of material used. A program was developed to generate these quantities when given experimentally-determined data for material density as a function of time at four hold temperatures. Three different small size CWF samples of 8, 200 and 500 grams were tested for calibration compatibility with large-scale samples. Using a linear potentiometer, consolidation levels were recorded over 60 hour hold periods at 875 degrees Celsius. All three sizes produced consistent data in multiple trials. The 500 gram sample, however, was found to have kinetic properties sufficiently similar to those of larger samples to assist in model calibration. It has been recommended that a full set of experiments at the four different hold temperatures be conducted using the 500 gram sample size.

Using a Micro Channel Plate for Beam-Line Imaging. AARON WITHERSPOON (*Morgan State University, Baltimore, MD 21251*) MARGARET MCMAHAN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The cyclotron has been running for over forty years. There have been many experiments done by the researchers at LBNL and by outside facilities. With a new interest in making radioactive beams it is necessary to develop more sensitive equipment. In addition, the cross sectional area of the beam as well as beam diameter have been unknown. The Micro Channel Plate (MCP) imaging detector allows the user to determine the shape and cross sectional area of the ion beam. In the past, the position of the beam that yields the best result could only be estimated. Multiple experiments were done using targets that cost thousands of dollars per gram. If the beam is not aligned properly with the target, then a good percentage of the beam is not utilized. With the use of the MCP detector, the ion beam can be positioned in such a manner that most of the beam provides maximum effect.

Developing a New Inner Vertex Detector for STAR: Characterizing an Active Pixel Sensor Prototype Chip. SAMUEL WURZEL (*Brown University, Providence, RI 02912*) HOWARD MATIS (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Identifying the Quark Gluon Plasma motivates the development of a new inner vertex detector for STAR. A vertex detector can measure the charmed component from heavy ion collisions. Active Pixel Sensor (APS) technology has been investigated as an alternative to Charged Coupled Devices (CCD) for use in the vertex detector because of its standard CMOS fabrication and radiation hardness. We have tested characteristics of a prototype APS chip with an array of 128x128 pixels. The chip is divided into sixteen 32x32 pixel sectors. The fabrication of pixel diodes in each sector is different in order to determine the most advantageous design. The bias and ground voltages of the pixel diodes were optimized to achieve maximal signal

to noise. We then cooled the chip and measured the leakage current across the pixel diodes and the signal to noise as a function of temperature. Since we plan to situate the inner vertex detector right outside the beam pipe, we tested the effect of 55 MeV protons from the 88" Cyclotron at LBNL. We exposed chips corresponding to the expected integrated dose seen at 40 times current RHIC luminosity over a period of 7 months to 30 years. We measured the increase in leakage current and decreased signal to noise as functions of dose.

PHYSICS

Spectroscopic Analysis of the SNS Ion Source. SACHIN BABU (*University of Texas, Dallas, Dallas, TX 75083*) ROBERT WELTON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

This project investigates the use of spectroscopy as an on-line diagnostic method of the SNS ion source plasma. Direct online measurements that can observe plasma density, monitor spectral lines associated with materials of the antenna coating, and track cesium in the source can greatly add to our understanding of the operation and failure mechanisms of an ion source. As a first step in developing these techniques, spectral measurements were taken during a 107 hr endurance test with the ion source at standard conditions. The data contained strong H Balmer lines and some peaks that indicated the presence of Cu, Ti, and Cs. The H line intensities (which are proportional to the plasma density) were shown to drop ~50% after 40 hrs into the endurance test, and rise ~30% after 70 hrs. The Cu, Ti, and Cs lines were shown to increase in the first 40 hrs of the endurance test, and remained stable thereafter. Electron temperature was estimated at ~0.4eV at the outer edge of the antenna; it remained constant for the entire endurance test. H⁻ current was measured to be ~6mA during the last few hours of the endurance test.

Spark Ignition Technology: Electric Arc Plasmas and Electrode Erosion. MATTHEW D'AMATO (*Ohio Wesleyan University, Delaware, OH 43015*) JOHN WHEALTON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

With interest in reducing automobile emissions and new technologies concerning internal combustion engine efficiency, we study the erosion of spark plug electrodes using fast imaging techniques and spectroscopy. High-pressure applications are particularly in need of spark plugs with low erosion rates. The design and implementation of a data acquisition system for obtaining photographic and spectroscopic electrode erosion information is discussed. The effects of spark plug gap and a 1500 gauss applied magnetic field (resulting in a rotating arc discharge) on electrode erosion are investigated. Work in progress is aimed at using orange and blue spectral lines emitted by the discharge as a measure of relative electrode erosion. Preliminary studies in air at atmospheric pressure and room temperature suggest that electrode erosion may be reduced by applying an external magnetic field to the discharge. Spectroscopic analysis and high-speed photography allow various aspects of the electric discharge to be imaged and studied in order to develop a better understanding of electrode erosion by arc discharges.

Goniometer Control System for Coherent Bremsstrahlung Production. VICTOR ACOSTA (*Augsburg College, Minneapolis, MN 55454*) PERRY ANTHONY (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

A system for the generation of a high-intensity, quasi-monochromatic photon beam is discussed. The theory behind coherent bremsstrahlung photon beam production is analyzed and developed. The mechanics of a goniometer control system are presented. The software developed for remote control of the goniometer is also discussed. Finally, the results from various performance measurements are included.

Measurement of Bunch Length of Relativistic Charge Particles using the Electro-optic Technique. MUSTAFA AMIN (*University of Texas, Arlington, Arlington, TX 76010*) THOMAS TSANG (*Brookhaven National Laboratory, Upton, NY 11973*).

The electro-optic technique offers a non-destructive way of measuring bunch length of relativistic charged particles down to the millimeter scale. In particular, T. Srinivasan Rao et al provide a single shot scheme to measure bunch length of sub millimeter electron bunches. In this scheme, the birefringence induced by the electric field of the

electrons converts the temporal characteristics of the bunch to a spatial intensity distribution of an optical pulse. For this scheme it is essential that the change in the spatial intensity distribution of the optical pulse be limited and correlated to the bunch length of the electron bunch. In this work an experimental correlation is established between a spatially varying electric field applied across an electro-optic crystal and the spatial modulation of the optical pulse probing this field in the crystal.

Plasma Filament Investigations Using High Speed Photography. STEPHEN ANDERSON (*Bethel College, Saint Paul, MN 55112*) ANDREW POST-ZWICKER (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

A Jacob's ladder apparatus and a plasma ball are two tools that are used to study plasmas in an educational setting. However, much of the physics behind these beautiful plasmas remain unknown or not well studied. A new way to examine these plasmas is through high-speed video imaging. We used a Canadian Photonic Labs Mega Speed 1000 camera to view behavior such as filament movement, fragmentation and recombination with other filaments at speeds at over 8500 frames per second. Analyzing our movies in slow motion, and through the aid of image processing software, we are able to trace each step of this behavior and quantify values such as filament brightness and thickness. Along with spectroscopic techniques, we infer basic plasma parameters and attempt to fully explain the physics controlling each source.

Automatic Alignment of X-Ray Beams. ZACHARY ANDERSON (*Carnegie Mellon University, Pittsburgh, PA 15213*) ANA GONZALEZ (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

Protein crystals and other biological samples diffract weakly in X-rays. It is therefore important that the X-ray beam be very stable. Cubic smoothing splines were fit to ion chamber counts versus the vertical position of the sample. The extrema, inflection points about the maximum, and other information about the spline were calculated to determine whether the data corresponded to a beam profile. The algorithm developed here correctly identified the absence of a beam profile in all data gathered over the course of a year from four beam lines at the Stanford Synchrotron Radiation Laboratory. This algorithm is effective and can be adapted to other beam lines.

Examination of New Ignition Concepts by Spectrographic and High Speed Photographic Technique. MARK BENNETT (*Jefferson Community Technical College System, Louisville, KY 40272*) JOHN WHEALTON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The use of natural gas as an alternative fuel in internal combustion engines has benefits of higher efficiency and lower emissions. However, the use of natural gas as a fuel requires higher engine compression ratios which results in accelerated sparkplug erosion and misfires do to the increase in capacitance at the sparkplug gap. Development of a method for testing sparkplug erosion instantaneously is under way. This new method will possibly allow for accelerated development of new ignition systems. A test cylinder has been designed to simulate pressures at which sparkplugs operate. The test chamber houses a quartz lens at one end which allows light emitted from a sparkplug arc to pass through to an optical setup into a spectrometer. The spectrometer houses a high speed Charge Injection Device (CID) camera that takes images from the arc spectrum and displays the image as a series of numbers representing average light intensity per pixel unit. Computer software is currently in design to manipulate the data received from the camera into a graphical form for ease of analysis, to analysis the ratio between an elemental peak and a volumetric peak and a method for averaging the area under the curve that may also provide erosion results. To have a testing apparatus that can give an amount of erosion instantaneously would be of great value for commercial development of improved ignition systems.

Nuclear Reaction Analysis of Helium Retention in 6H-SiC as a Function of Irradiation and Annealing. LUKE BISSELL (*Brigham Young University, Provo, UT 84602*) THEVA THEVUTHASAN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Silicon carbide and silicon carbide composites have been proposed as cladding material in advanced gas-cooled and light water reactors. As such, the effects of irradiation and fission gases on the performance of SiC in the reactor environment are critical in several ways. Since He

serves as a cooling gas, low-energy He (< 50 keV) will be colliding with the outer surface cladding layers. Furthermore, it is also one of the fission products. Thus, it is important to understand He retention in SiC under advanced reactor operating conditions. We investigated He retention in single crystal 6H SiC as a function of irradiation dose and annealing temperature using nuclear reaction analysis (NRA) via the $3\text{He}(\text{D},\alpha)^1\text{H}$ reaction. Helium ions with 40 keV energy were implanted in the SiC to a depth of ~360 nm at room temperature under high vacuum conditions. The samples were then transferred to another high vacuum chamber where the NRA was performed using a 1.0 MeV D⁺ beam. Helium retention was studied as a function of D⁺ irradiation dose at 300 K from 1.4×10^{16} to 12.5×10^{16} D⁺/cm², and as a function of annealing temperature ranging from 300 - 1600 K. No significant helium loss was observed due to irradiation, and only annealing temperatures above 1400 K caused measurable loss of helium. These results will be discussed along with the details associated with the $3\text{He}(\text{D},\alpha)^1\text{H}$ nuclear reaction.

Optimizing Small Molecular Crystallography. ARNESTO BOWMAN (*Fisk University, Nashville, TN 37208*) AL THOMPSON (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*). The study of small-sized crystals of molecular compounds has become a major focal point of biological and chemical research. With this advance in focus, the mission of developing new techniques to study these very small samples has also become vital. Beamline 11.3.1 of the Advanced Light Source at Lawrence Berkeley National Laboratory has stepped up to the challenge of this task. The beamline takes advantage of the high flux of synchrotron radiation sources and ingenious beam focusing optics to provide for the measurement of X-ray diffraction patterns of crystals that are tens of times smaller than can be achieved in a conventional laboratory. The author's task on this new beamline was to measure the X-ray diffraction intensity data, and determine the crystal structures of, cobalt hexaimidizolate and copper hexaimidazolate. Problems with the synthesis of these compounds were discovered upon the successful solution and refinement of the data collected. This research led to the confirmation of the performance goals of the beamline.

Charge Carrier Generation and Exciton Quenching at M3EH-PPV/Small Molecule and M3EH-PPV/Oxide Interfaces. KATHRYN BROWN (*Colorado School of Mines, Golden, CO 80401*) DAVID GINLEY (*National Renewable Energy Laboratory, Golden, CO 89401*). The need for efficient exciton dissociation is one of the most important factors limiting improved efficiencies in organic photovoltaic devices. Using luminescence as a probe, we studied the quenching of excitons in semiconducting polymers for a variety of quenching materials, including transparent conducting oxides (TCOs) and small molecule perylene diimide thin films. Perylene benzimidazole (PBI) is shown to be the best quencher of those studied. This result is consistent with the improved conversion efficiencies demonstrated when this material is used in a polymer bilayer photovoltaic device.

Stability Properties of the RMS Envelope Equations Describing Intense Ion Beam Transport. BORIS BUKH (*City College of San Francisco, San Francisco, CA 94112*) STEVEN M. LUND (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*). Accelerator based drivers for heavy ion fusion require multiple ion beams with high space-charge intensity. Such ion beams are typically transported in a periodic lattice of alternating gradient quadrupole magnets that focus (confine) the beam. The low-order transverse evolution of the mid-pulse envelope of beam particles in periodic quadrupole focusing channels is described by the so-called Kapchinskij-Vladimirskij (KV) envelope equations. It is imperative that practical transport channels be designed where the matched (i.e., periodic) beam envelope is linearly stable. Here we present a parametric stability analysis of the KV envelope equations for quadrupole lattices with equally spaced quadrupole lenses (symmetric FODO) and staggered (syncopated) lenses. Numerical analyses of scaled envelope equations are performed to parametrically map boundary regions of unstable envelope bands, thereby providing important, practical data for transport channel design. Parametric sensitivities are explored and a previously unanticipated envelope instability is found for syncopated quadrupole lattices. Numerical results re compared to thin-lens (i.e., axially short quadrupoles) results

in the limit of weak and strong space-charge corresponding to undepleted and fully depleted beams.

Development of Error Generation and Correction Models for the ORBIT Accelerator Beam Dynamics Code. STEVEN BUNCH (*University of Tennessee - Knoxville, Knoxville, TN 37919*) JEFF HOLMES (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*). Issues of beam dynamics in the SNS accumulator ring are studied using ORBIT (Objective Ring Beam Injection and Tracking), a C++ object-oriented particle tracking code for accelerator rings. One of the top priorities in ORBIT development is the creation of models to simulate magnet alignment errors, both to ascertain and to correct their effect on beam transport and losses. The project here was to develop and test a number of models for magnet errors and their correction in ORBIT. Development was done in Linux using the GNU g++ compiler and text editors. Three different modules were developed, an Error module, a Closed Orbit module, and an Error Correction module. The Error module consists of general coordinate displacement routines, a routine to generate individual magnet displacement errors, a routine to generate sets of randomly distributed magnet errors, and a routine to display the errors. The Closed Orbit module consists of one routine that calculates the closed orbit solution for the ring, which is important in the presence of errors. The Error Correction module contains one routine which adds a beam position monitor and a dipole corrector magnet. The monitor and corrector work in conjunction to minimize beam excursions in the ring. All three modules are essential to the description and correction of magnet errors using ORBIT, and hence necessary for achieving extremely low beam losses. The addition of these modules gives the accelerator physicists critical insight into how errors affect ring dynamics and what can be done to correct them.

Spectral Analysis of Lower Hybrid Magnetic Fluctuations in the Magnetic Reconnection Experiment. JOSHUA CARTER (*The University of North Carolina at Chapel Hill, Chapel Hill, NC 27514*) HANTAO JI (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*). Magnetic reconnection, the topological annihilation and reconnection of magnetic field lines, is a crucial process occurring in both astrophysical and laboratory plasmas evident in solar flare creation and magnetically confined fusion. The Magnetic Reconnection Experiment (MRX) directly observes the reconnection process in a laboratory setting, focusing on a wide array of electrostatic and magnetic instabilities. One class of micro instabilities, which may be described as electromagnetic Lower Hybrid Drift Instabilities (LHDI), is currently under scrutiny as a source of explanation for fast reconnection (anomalous resistivity). The objective of the present study is to use spectral analysis techniques to find coherence lengths for the observed magnetic fluctuations to better characterize their linear and nonlinear behaviors. Detailed results will be presented together with comparisons with theoretical predictions. References P. Yoon et al., *Phys. Plasmas*, vol.9, 1526 (2002).

Improvements and Additions to Support Systems of Atlas ECR Ion Sources. THOMAS CECIL (*Murray State University, Murray, KY 42071*) RICK VONDRASEK (*Argonne National Laboratory, Argonne, IL 60439*). The Atlas facility is a national user facility that provides heavy-ion beams for use in a wide variety of experiments. The facility consists of two ion injector sites, booster linac sites, and several target experimental sites. The facility is capable of producing ion beams from as light as helium to as heavy as Uranium in high charge states. The starting point for any ion beam is the ion source. The positive ion injector has two Electron Cyclotron Resonance ion sources (ECRI and ECRII). Keeping the ECR sources properly running requires numerous support systems. Some of these systems include cooling water, power supplies, support gas supply, and safety controls. My project this summer will involve the upgrade and maintenance of several of these systems. Projects currently in progress are 1) an expanded electrical safety cage for ECRII, 2) a more robust deionized cooling water system for ECRI, and 3) a support gas handling system for both ECR sources. The safety cage on ECRII is being expanded to ensure complete enclosure of the source with the addition of a capture key lock. An increase of cooling power from the existing 45 kW to 125 kW for ECRI involves replacing the existing cooling-water circulation pump and heat exchanger, and installing new water circulation piping. A gas

handling system for both ECR sources is to be designed and built. The system will allow for alternating between three support gases without breaking the vacuum of the source.

Developing a Measurement of Secondary Electron Emission from Ion Bombardment. ADAM COOREY (*University of California, Los Angeles, Los Angeles, CA 90095*) ART MOLVIK (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Accelerators for heavy-ion inertial fusion energy (HIF) have an economic incentive to fit beam tubes tightly to beams, putting them at risk from electron clouds produced by secondary electrons, and ionization of gas from walls. We are beginning studies on the High-Current Experiment (HCX) to characterize electron production and trapping, the effects on ion beams, and mitigation techniques. We measured the flux of electrons and gas evolved from a target, whose angle to the beam can be varied between 2 degrees and 15 degrees from grazing incidence. We determined the secondary emission varies as the $(\cos(\bar{E}))^{-1}$ where \bar{E} is the angle of incidence. Although the beam current could not yet be directly measured, we estimated it to determine approximate secondary emission coefficients varying from 40 to 185 with the angle of incidence. We have built a simple Faraday cup to measure the beam current directly.

High Energy Elastic Electron Scattering Cross Sections from 3He. JUAN CORNEJO (*California State University at Los Angeles, Los Angeles, CA 90032*) ARUN SAHA (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

Part of the E89-044 experiment conducted at the Thomas Jefferson National Accelerator Facility's experimental Hall A studied the electron elastic scattering cross section off 3He nuclei with two independent analyses. The two analyses revealed a discrepancy at low values of four momentum transferred squared (Q^2). This report presents results from an ongoing third analysis attempting to understand the discrepancy. This analysis will focus on four specific details of the previous analyses that resulted in distinct results.

Lecture SLAC-PUB-9380. CYNTHIA CORREA (*Harvard University, Cambridge, MA 02138*) GRZEGORZ MADEJSKI (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

We report results of hard X-Ray observations of the clusters Coma, Abell 496, Abell 754, Abell 1060, Abell 1367, Abell 2256 and Abell 3558 using RXTE data from the NASA HEASARC public archive. Specifically we searched for clusters with hard x-ray emission that can be fitted by a power law because this would indicate that the cluster is a source of non-thermal emission. We are assuming the emission mechanism proposed by Vahé Petrosian where the inter cluster space contains clouds of relativistic electrons that by themselves create a magnetic field and emit radio synchrotron radiation. These relativistic electrons Inverse-Compton scatter Microwave Background photons up to hard x-ray energies. The clusters that were found to be sources of non-thermal hard x-rays are Coma, Abell 496, Abell 754 and Abell 1060.

Forward Calorimeter for the Muon Arm Upgrades at PHENIX. KELLY CORRIEA (*University of California, Riverside, Riverside, CA 92521*) MATTHIAS GROSSE-PERDEKAMP (*Brookhaven National Laboratory, Upton, NY 11973*).

The Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) was commissioned for polarized proton collisions. In the coming years, data collected at RHIC is expected to address many unanswered questions on the topic of nucleon spin. One important topic which will be addressed by running RHIC at $\sqrt{s}=500\text{GeV}$ is the contribution of different flavors of quarks and anti-quarks to the nucleon's spin. Understanding this can be achieved via production of W bosons in polarized pp collisions and their subsequent weak decays into leptons. The PHENIX detector will make this measurement with W particles decaying into muons using muon arms with a rapidity acceptance of 1.2 to 2.4. However, at the RHIC design luminosity, the muon trigger rate is expected to be 20kHz, well beyond the expected bandwidth available in the data acquisition system for this physics channel. A significant amount of this rate comes from decays of pions and kaons produced by background reactions. One proposal for suppressing this background at the trigger level is to replace the inactive absorber material in front of the muon arms with an active electromagnetic calorimeter. Using Monte Carlo simulations of such a calorimeter, we studied event topologies of the W and QCD back-

ground events to determine possible parameters for differentiating between the events.

Characterization of Ti: Sapphire Laser Rods for Installation in the Polarized Light Source. SEAN CORUM (*Augustana College, Sioux Falls, SD 57197*) AXEL BRACHMANN (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

The Flash:Ti laser in the Polarized Light Source at the Stanford Linear Accelerator Center (SLAC) is used to obtain spin polarized electrons for high-energy particle physics experiments. The Flash:Ti laser utilizes titanium-doped sapphire (Ti:Sapphire) crystals to produce laser light. The properties of these crystals, or laser rods, greatly affect the quality of the laser beam produced (e.g. power and jitter), which in turn affects the overall quality and reliability of the particle physics experiments at SLAC. In this interest, seven Ti:Sapphire laser rods were tested for absorption and transmission properties as a function of angular position (i.e., the rod was rotated along its geometrical axis). 833 nm light from a diode laser was linearly polarized and passed through the rods to test for transmission properties. The time-averaged power output of the emitted light was measured with a photodiode/powermeter apparatus. Similarly, the absorption properties of the rods were tested by passing linearly polarized light from a 543 nm green He:Ne laser through the rods. The rod with the best combination of absorption and transmission properties was selected for installation in the Polarized Light Source at the Stanford Linear Accelerator Center.

Partial Discharge in Solid Epoxy at Room and Cryogenic Temperatures. DANIEL DESCHENES (*California State University Fresno, Fresno, CA 93710*) ISIDOR SAUERS (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Partial discharges (PD) are small surges of current, which occur generally in manufacturing defects in an electrical insulation system when the applied voltage exceeds a threshold value. Such undesirable discharges can over time deteriorate the insulation and shorten the lifetime of equipment resulting in a catastrophic, costly, and unpredictable failure. Therefore, understanding PD and its causes can help diagnose problems and predict the expected lifetime of a dielectric. For cryogenic insulation used in High Temperature Superconducting power equipment applications such as cables, transformers, and fault current limiters, PD is thought to be the primary degradation mechanism of the electrical insulation. One of the more common defects in a dielectric insulator is a spherical void that forms as a bubble in the curing of an epoxy. To study the pattern of PD, samples were prepared with artificial voids embedded in epoxy between parallel plane electrodes. The PD signal was investigated as a function of magnitude and phase angle of applied voltage using a commercial digital PD detector with a sensitivity range from as low as 1 Pico-Coulomb(10-12 C) to several Nano-Coulombs(10-9 C). Different PD "signatures" are observed for samples with a different number of voids, and from the same sample at room and cryogenic temperatures. In order to help clarify the PD signals originating only from the sample, other sources of PD are discussed, along with noise and techniques to reduce this noise.

Comparison of Two Wire Chamber Track Reconstruction Algorithms used in Hall A at Jefferson Lab. SEAN DOBBS (*Carnegie Mellon University, Pittsburgh, PA 15213*) JENS-OLE HANSEN (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

The Hall A collaboration at Jefferson Lab is currently in the process of redesigning and rewriting its physics analysis software in C++, using the ROOT libraries developed at CERN, to replace the Fortran-based ESPACE analyzer. In this paper, we carry out a detailed comparison of the wire chamber tracking results of both software packages. To this end, reconstruction of target quantities from detected tracks through the Vertical Drift Chambers (VDCs) in both spectrometer arms has been recently added to the C++ analyzer, to bring it to the same level as ESPACE. A study of the differences in the outputs of both analysis programs shows that while the output of the C++ analyzer is suitable for calibrations and studies that do not require high resolution, there are still many subtle differences that need to be resolved before it is ready for a production-quality release. The problems are most likely due to different cluster matching and track fitting algorithms used by both programs for tracks through the VDCs, as well as certain corrections missing from the C++ code. These problems and some possible solutions are discussed.

Development of a Systems Analysis Education Module using Web-Based Instructional Tools. JENNIFER DOCKTOR (North Dakota State University, Fargo, ND 58105) PAUL MADSEN (Fermi National Accelerator Laboratory, Batavia, Illinois 60510).

As technology continues to expand at a rapid rate, the world is becoming increasingly dependent upon complex computer hardware and software systems. What happens when these systems fail? There is a need for the general public to have a fundamental understanding of how to analyze systems to predict and handle potential system problems. This is a description of the development process and contents of a web-based education module in which students will explore the central topics of systems dependability. Activities include building a Rube Goldberg device and analyzing satellite telemetry data sets, among others. A special format called WebQuest was utilized to develop the lesson into a web page, which is a unique inquiry-oriented model that is designed to make wise use of learners' time by focusing students on the information itself and not on searching for it. The core structure of the website consists of introduction, task, process, evaluation, conclusion, and teacher pages. Trials by educators in the field will be the true test of the effectiveness of this web-based systems analysis module.

Computer Interactive Display Demonstration. TINA DREW (University of Maryland Eastern Shore, Princess Anne, MD 21853) ANDREW POST-ZWICKER (Princeton Plasma Physics Laboratory, Princeton, NJ 08543).

The goal of my research project this summer was to make a computer interactive, plasma display demonstration that will be used to teach high school and college students. This model will be used to educate the community about plasma properties. By informing the public about plasma, we will increase common knowledge of and interest in plasma. This will allow people to see plasma as a more attainable source of energy. My demonstration will be computer interactive and allow the user to control and explore plasma parameters. It will also demonstrate magnetic confinement. It will be a representation of the intertwining of modern technology and teaching plasma physics.

Measurement Lifetime of Muons in Matter. DAVID FIGUEROA (University of Puerto Rico Mayagüez Campus, Mayagüez, PR 00680) HELIO TAKAI (Brookhaven National Laboratory, Upton, NY 11973).

The Fermi constant G_F is one of the fundamental parameters in the Standard Model. It governs the strength of any electroweak process. The muon decay rate is related to G_F by the expression $\Gamma_{\text{muon}} = (1/\tau_{\text{muon}}) = ((G_F m_{\text{muon}}^5 / 192 \pi^3)) (1+d)$ where the term d represents QED radioactive corrections. With a thorough review of the relationship between τ_{muon} and G_F , the theoretical error has been reduced to less than 0.1ppm. This advance coupled with increased muon beam fluxes and beamline development opens the door for a new high-precision measurement of the muon lifetime, and thus a new determination of G_F . This effort has the goal of measuring τ_{muon} to a precision of 1 part in 10^8 giving an absolute uncertainty on the level of 2ps and a new value for G_F with a precision at the 0.5ppm level. This represents a 20-fold improvement compared to the current world average. Complementary examples include the enormous effort expended at CERN to determine the Z-boson mass to 2MeV(22ppm), new data on the W mass which will lead to a determination at the few hundred ppm level and improved extrapolation of the running of the fine-structure constant to the Z-mass pole. Future linear or muon colliders will aim at significant improvements in these quantities, as will current higher-precision determinations of the $e^+e^- \rightarrow \text{hadrons}/\mu\text{ons}$ R ratio over a broad range of \sqrt{s} . Already, the low q^2 knowledge of α is at the 0.004 ppm level using the results from electron $g_e - 2$ measurements and plans are underway to decrease the error on α by a factor of 10. It is our belief that measurements of the fundamental constants, which can be performed with great precision, will be of enduring value.

Construction of a Large Gas-cell Catcher Prototype for the Collection of Fast-recoiling Fragmentation Products. ADAM FRANKEL (Cornell University, Ithaca, NY 60089) GUY SAVARD (Argonne National Laboratory, Argonne, IL 60439).

By incorporating a large gas-cell catcher into a high-power version of a fragmentation-based ISOL, it will be possible to thermalize and extract ions for post-acceleration and thereby attain simultaneously the quality and precise energy of an ISOL system and the universality and short delay time of a fragmentation-based system. A prototype

gas-cell catcher along with the circuit that controls it has been constructed for this purpose and preliminary tests of the electronics have been performed. It has been determined that the electronic circuit of the accelerating section of the gas cell behaves according to the specifications (determined from simulations) that will be necessary for it to perform its intended function. The next step will be to test the circuit of the focusing section. Following that, some tests of extraction efficiency and delay time will be performed with the prototype using low-energy ions produced at the ATLAS facility at Argonne National Laboratory. Finally, the prototype will be tested at a higher energy behind the fragment separator at GSI in Germany to determine its viability as a new piece of technology for a next generation radioactive beam facility called RIA.

Energy Analyzers for Helicon Plasma Source-Driven Rocket Engine. RYAN GIAR (University of Tennessee - Knoxville, Knoxville, TN 37916) DAVE RASMUSSEN (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The variable specific impulse magneto-plasma rocket (VASIMR) is a novel propulsion concept pioneered by Franklin R. Chang Diaz. To calculate thrust from such an engine one requires knowledge of the mass flow rate of the propellant (in this case a highly ionized plasma) and the kinetic energy of the propellant particles. The latter parameter is the focus of the experimentation in Oak Ridge's scaled-down radio frequency test facility (Mini-RFTF) for the VASIMR engine. The plasma energy is measured using retarding potential analyzers (RPA). An RPA is a device that consists of parallel grids and a collector plate. A plasma beam is created with a helicon source and directed through grids of varying voltage bias and strikes the collectors. The grids repel electrons, and the current from the collectors indicates the energy of the ions (differentiating current with respect to voltage equals energy). Studies with the RPA have yielded data about plasma temperatures and heating. Mini-RFTF has shown plasmas with ion energies and densities higher than predicted by theory or similar experiments. Thus the bulk of the work done with the RPA's in Mini-RFTF has involved changing design parameters to verify the correct operation of the analyzer. Preliminary measurements indicated the need for radio frequency filters and reduced grid hole sizes. To accommodate the high ion density the grid hole size was reduced to $\sim 80\mu\text{m}$ which corresponds to two plasma Debye lengths. Radio frequency choke filters were added to the collector plate substrate. Tests were also conducted on miniature solid-state analyzers; those results are presented.

The Design of an Interdisciplinary Experiment: Cellular Ion Transport and Similarities to Plasma Physics. JENNIFER GIMMELL (Hiram College, Hiram, OH 44234) ANDREW POST-ZWICKER (Princeton Plasma Physics Laboratory, Princeton, NJ 08543).

A recent theoretical publication in the American Journal of Physics [1] compares a mathematical model of plasma double layers to experimental data of ion transport across cell membranes. There exists a measurable voltage difference between a cell's internal cytoplasm and the external cellular material that causes a double layer to form between the cytoplasm and the bio-plasma. Similarly, when studying two plasmas of different cross sectional areas, a double layer in the plasma forms on the interface between the two separate volumes. Applying the knowledge and information gained in several glow discharge and Langmuir probe experiments, we design an experiment that investigates the fabrication of double layers and makes connections between experimental data and biological ion transport across cell membranes. [1] M. Uehara, K. K. Sakane, H.S. Maciel and W.I. Urruchi, "Physics and Biology: Bio-plasma physics," Am. J. Phys. 68 (5), 450-455 (2000).

Muon Trigger Upgrade for PHENIX. JACOB GORDON (Harvard University, Cambridge, MA 02138) GERRY BUNCE (Brookhaven National Laboratory, Upton, NY 11973).

Experiments with high energy, polarized protons at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory will produce data allowing new insights into the spin structure of the proton. The parity violating nature of the electroweak force enables a direct measurement of the spin contribution of individual flavors of quarks and anti-quarks via the W production channel. To date, no such measurement has been made. The PHENIX detector at RHIC is capable of detecting muons from the decay of W bosons in the pseudo-rapidity range from 1.2 to 2.4. These muons, however, are obscured by soft

muon production from hadron decays. For polarized proton collisions at the expected luminosity, the current muon trigger cannot sufficiently filter the desired, higher momentum muons (>10 GeV) from the muons in the background (~ 2 GeV). We studied three proposals for upgrading the PHENIX detector. First, we studied the use of a new hodoscope with which tracks through the magnetic field could be reconstructed in real time. Second, we investigated the addition of a threshold Cherenkov counter for distinguishing high momentum muons. Finally, we studied the utility of using a nosecone calorimeter to distinguish events based on topological differences. Simulation results studying feasibility and design considerations will be presented.

Preliminary Study of $D_0 \rightarrow K\pi\pi_0$ Decays with Dalitz Plots.

MOIRA GRESHAM (Reed College, Portland, OR 97202) RAY COWAN (Stanford Linear Accelerator Center, Stanford, CA 94025). Particle physicists study the smallest particles and most basic rules of their interactions in humankind's current scope. The Charm Analysis Working Group (CWG) of the BaBar Collaboration studies decays involving the charm quark. They currently study mixing in D decays, an interesting and poorly understood phenomenon in current physics models. We, as part of the CWG, investigated the plausibility of using Dalitz plots and the BaBar analysis framework to study mixing in Wrong Sign (WS) $D_0 \rightarrow K\pi\pi_0$ decays. Others in the CWG have studied mixing in the 2-body decay, $D_0 \rightarrow K\pi$. The 3-body decay analyzed with the RooFitDalitz analysis package and Dalitz plots provides more information and another way of separating Doubly Cabibbo Suppressed Decays (DCSD) from mixing — which share the same end products. Through doing many simulations, we have demonstrated the usefulness of this approach. We selected $D_0 \rightarrow K\pi\pi_0$ events from Simulation Production run #4 (SP4) and BaBar's run 1 and run 2. We made Dalitz plots with this data. Now that we better understand Dalitz plots and software, we plan to select WS $D_0 \rightarrow K\pi\pi_0$ events and perform rate fits as discussed in BaBar Analysis Document (BAD) #443, as well as fits for several different decay times and resonances, in order to further distinguish DCSD from mixing.

Ultra-sensitive Atom Trap Trace Analysis of Calcium Isotopes.

WILLIAM GRIMES (Monmouth College, Monmouth, IL 61462) ZHENG-TIAN LU (Argonne National Laboratory, Argonne, IL 60439). Atom Trap Trace Analysis (ATTA) is an ultra-sensitive method capable of trapping, detecting and counting single atoms of long-lived radioactive trace isotopes. The method, based on a magneto-optical trap has been used to trap isotopes of krypton and calcium. ^{81}Kr has a half-life of 2.3×10^5 years (and an abundance of 6×10^{-13}) making it the ideal isotope for dating ancient ground water and ice on the order of one million years. ^{41}Ca , with a half-life of 1.03×10^5 years and an isotopic abundance of $\sim 10^{-15}$, has promising applications as a biomedical tool to directly measure the loss of bone mass (osteoporosis). Counting ^{41}Ca ratios in samples of old bone could lead to the dating of archeological findings on the order of 105 years, improving our understanding on the early origins of life. These methods are relatively new and much research is concurring to provide a practical system for real-life applications. This summer I have worked on a daily basis with the ATTA Ca setup. We have been successful in producing a trap sensitive enough to detect single atoms of all stable calcium isotopes. I spent my time working to improve the sensitivity of the trap and therefore increasing the probability of detecting single atoms of the extremely rare isotope, ^{41}Ca . I have been working with our detection system, to continually improve the signal to noise ratio of the fluorescence of a single atom.

Reconstructing Total Photon Energy and Direction in a Germanium Detector. *SEAN GRULLON (Florida International University, Miami, FL 33199) TENG LEK KHOO (Argonne National Laboratory, Argonne, IL 60439).*

A photon entering a detector and interacting at different points can be reconstructed using a computer program. The algorithm in the program was made to determine all the valid incoming photon energies and display them on a histogram to give a spectrum. The program tracks gamma rays from specific location and rejects photons not coming from a radioactive source at a specified location. It is important to track the incoming photons and reject the dominant background photons coming from a location other than the radioactive source. The program was done using ROOT, a new data acquisition, visualization, and analysis package with an included C++ interpreter. Artificial data was created with this package as well to test the abilities of the program.

The program takes the correctly identified incoming photons, graphs them on a histogram, and graphs the rejected photons on another histogram. The next step in for the program is to analyze data created in a Monte Carlo simulation, and eventually use the data in conjunction with an actual experiment.

The BigBite Spectrometer. *CHARLES HANRETTY (Florida A&M University, Tallahassee, FL 32307) DOUG HIGINBOTHAM (Thomas Jefferson National Accelerator Facility, Newport News, VA 23606).*

In order to increase the experimental capabilities of Hall A, the construction of a third spectrometer called BigBite is underway. This "third arm" will greatly add to the Hall's capability of detecting scattered subatomic particles. This new spectrometer has a very broad kinematic coverage as result of the spectrometer's large momentum and angular acceptance. BigBite will provide data which is complementary to that collected by the High Resolution Spectrometers. By vacuum coupling BigBite to the Hall's scattering chamber, the new spectrometer will readily be able to detect the passing of low-energy protons scattered as a result of the quasi-elastic scattering. In this work, CAD drawings of the new spectrometer's detectors and the test setup will be presented.

Characterization and Calibration of KOPIO Micro-bunching Detector/Monitor Prototype. *SONDRA HELLSTROM (Johns Hopkins University, Baltimore, MD 21218) MICHAEL SIVERTZ (Brookhaven National Laboratory, Upton, NY 11973).*

The decay of a neutral kaon into a neutral pion and neutrino anti-neutrino pair has one of the most straightforward direct charge parity violation mechanisms known; precise measurement of its branching ratio provides a stringent test of the standard model and opportunity for observation of new physics. For adequate kaon time-of-flight measurements using the Alternating Gradient Synchrotron (AGS), RF pulse width in a spill must be 250 ps or less with 40 ns between pulses. A prototype for measurement and monitoring of these RF pulses, consisting of a series of telescope scintillators and veto counters with an aerogel Cherenkov counter, is tested using a test beam from the AGS as well as cosmic rays. In the test beam, veto counter efficiency is measured at 99.98%; this value becomes 99.995% when restricted to low-momentum charged tracks. Cosmic ray muons are detected at nearly 100% efficiency. A consistent efficiency difference between the veto counters is partially explainable by photon pair production in the first counter. Timing shift between low and high pulse height events is typical of discriminator usage. The minimum ionizing particle (MIP) response varies from 32 to 112 pC for cosmic rays with the photomultiplier tube voltages varying over 100V. Total gain is on the order of 10^6 , slightly lower than theoretically predicted. Cherenkov counter pulse height responses are determined to be reasonably dependent on stimulation frequency, less dependent on amplitude, and seem to be vulnerable to high singles rates and accidentals; future experimentation in this area is necessary.

Muon Trigger Upgrades for PHENIX. *JENNIFER HOM (Columbia University, New York City, NY 10027) ABHAY DESHPANDE (Brookhaven National Laboratory, Upton, NY 11973).*

Experiments with high energy, polarized protons at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory will produce data allowing new insights into the spin structure of the proton. The parity violating nature of the electroweak force enables a direct measurement of the spin contribution of individual flavors of quarks and anti-quarks via the W production channel. To date, no such measurement has been made. The PHENIX detector at RHIC is capable of detecting muons from the decay of W bosons in the pseudo-rapidity range from 1.2 to 2.4. These muons, however, are obscured by soft muon production from hadron decays. For polarized proton collisions at the expected luminosity, the current muon trigger cannot sufficiently filter the desired, higher momentum muons (>10 GeV) from the muons in the background (~ 2 GeV). We studied three proposals for upgrading the PHENIX detector. First, we studied the use of a new hodoscope with which tracks through the magnetic field could be reconstructed in real time. Second, we investigated the addition of a threshold Cherenkov counter for distinguishing high momentum muons. Finally, we studied the utility of using a nosecone calorimeter to distinguish events based on topological differences. Simulation results studying feasibility and design considerations will be presented.

Testing Fiber Optic Cables at 300 and 4.2 K. *FAWN HUISMAN (Reed College, Portland, OR 97202) JOHN WEISEND (Stanford Linear Accelerator Center, Stanford, CA 94025).*

Strange "cavity lights" have been observed in Superconducting Radio Frequency (SCRF) Cavities. In order to understand this phenomenon a spectral analysis of the light is necessary. However, the extreme conditions presented within the cavity require the equipment to function at cryogenic temperatures. Ocean optics P600 UV/VIS fiber optic cables were studied at 300 K and 4.2 K to determine whether or not they would be appropriate for cryogenic temperatures. At 300 K the performance of different lengths of cable, the effect of a lens and the effect of a junction were investigated by taking spectra of red, green, and yellow LEDs at a variety of distances from where the source and the cable/spectrometer were aligned. It was found that there was significant attenuation of the signal between the spectrometer alone and the spectrometer with any combination of cables. The lens reduced the number of locations where a readable signal was produced, but the intensity increased greatly when the lens was aligned with the light source. The junction did not seem to make a difference except when there was a large angle between the light source and the cable. At 4.2 K a 4 m cable and a lens were submerged in liquid Helium to test their capabilities at cryogenic temperatures. The fiber optic cable was found unsuitable for use as it did not function at 4.2 K, and the signal was essentially lost. However, the lens survived.

Automatic Precision Measurements of Planar Angles.

JONATHAN HYMAN (Wake Forest University, Winston-Salem, NC 27109) BOGDAN WOJTSEKHOWSKI (Thomas Jefferson National Accelerator Facility, Newport News, VA 23606). Inside Hall A at the Thomas Jefferson National Accelerator Facility, two large spectrometers observe and measure electrons after they collide with the target. The analysis of nuclear reactions requires that the angle between the incident electron beam and bending magnets of the spectrometer be known. Presently, this angle is measured by a survey crew with theodolites, thus requiring the beam to be shut off. The innovation of an automatic angle measurement device was developed to improve the current process by allowing the same measurements to be taken without sacrificing vital beam time. Lasers directed onto spinning devices positioned on the walls inside Hall A create revolving horizontal beams of light that are recorded by various photon detectors located on the spectrometers. From a conversion of time intervals between light pulses to angles, the angles separating photon detectors are measured for determining the angle between the incident electron beam and bending magnets within an accuracy of 0.1 milliradian. Through the designing of a spindle, a relative angular stability of 1×10^{-5} was achieved, thus resulting in an angular accuracy of 0.03 milliradians.

Fabrication and Optimal Positioning of Beam Loss Monitors.

DAVID JOHNSON (Virginia Polytechnic Institute and State University, Blacksburg, VA 24060) KEVIN JORDAN (Thomas Jefferson National Accelerator Facility, Newport News, VA 23606). The Free Electron Laser Facility at Thomas Jefferson National Accelerator Facility is currently being upgraded to a 10 kW infrared laser. Within the context of this upgrade there is a need for an upgrade of the Machine Protection System (MPS). Because of the near 2 MW power in the electron beam, there is a need for relatively fast monitors that will detect beam loss throughout the accelerator. In the event that the electro magnets used for steering the beam become corrupt, of other problematic occurrences in instrumentation, the beam will lose accuracy (in direction) and focus thus creating a major problem. Because such damage could occur on the order of milliseconds, highly sensitive radiation sensors were chosen. Taking sensitivity and cost into account the Burle 931B Photo multiplier Tube was chosen. The casing and electronics were then assembled according to an already used design; the result was finished Beam Loss Monitors (BLMs). Once the BLMs were fabricated, they were tested for their response. The BLM gain curves were consistent with the manufactures specification and MPS requirements. Once these results were obtained, an investigation began to find the most useful places along the beam line for the BLMs. This was done using an Excel spread sheet simulation of FEL. When using this simulation, three major considerations were taken into account to find the places where beam loss is most likely to occur: beam response to steering, beam size and aperture of vacuum cavity. The simulation showed places where beam

loss was most likely to occur. Finally, the cabling was installed along the FEL according to the positions suggested by the simulation.

Amplifying High-Frequency Acoustic Signals. *CARMEN KUNZ (San Jose State University, San Jose, CA 95192) JOE FRISCH (Stanford Linear Accelerator Center, Stanford, CA 94025).*

In search of the hypothetical Higgs boson, a prototype electron accelerator structure has been developed for use in the Next Linear Collider (NLC), SLAC's proposed version of the machine necessary to create the predicted particle. The Next Linear Test Accelerator (NLCTA), designed to provide 0.5 GeV - 1 TeV center-of-mass collision energy, generates electromagnetic breakdowns inside its copper structure while the beam is running. The sparks vaporize the surface of the copper, and will eventually ruin the accelerator. They also create high-frequency (hf) acoustic signals (100 kHz - 1 MHz). Acoustic sensors have been placed on the structure, however current knowledge regarding sound propagation in copper limits spark location to within one centimeter. A system was needed that simulates the sparks so further study of acoustic propagation can be pursued; the goal is locate them to within one millimeter. Various tests were done in order to identify an appropriate hf signal source, and to identify appropriate acoustic sensors to use. A high-voltage spark generator and the same sensors used on the actual structure proved most useful for the system. Two high-pass filters were also fabricated in order to measure signals that might be created above 2 MHz. The 11-gain filter was used on the acoustic simulation system that was developed, and the 100-gain filter will be used on the NLCTA.

Investigation of Ceramic Matrix Composites for Applications in Superconducting Magnets. *ANDREW LAFORGE (University of Puget Sound, Tacoma, WA 98406) STEVE GOURLAY (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

As superconducting magnets are being developed to meet the demands of new accelerator designs, existing systems are being scrutinized to reach optimal performance. Ideally, each component of the magnet is being pushed to the intrinsic limits of its constituent material. Ceramic matrix composites have been investigated for possible use in the fabrication of magnet coil end spacers. Several fabrication methods have been examined, and we see that favorable properties in handling, resistivity, and compatibility can be gained without making a large sacrifice in elastic modulus.

Development of Numerical Solutions to Laplace's Equation on Unstructured Grids. *BRIAN LAMARCHE (Washington State University, Pullman, WA 99163) GREG SCHENTER (Pacific Northwest National Laboratory, Richland, WA 99352).*

Representing solvent-solute interactions of condensed phases as a dielectric continuum model for understanding chemical equilibria is an engaging computational process. An infant technique using unstructured meshes to find electrostatic potentials and fields is in development. Finding the potentials on the mesh is done by solving Laplace's equation at every node on the mesh and completing an iterative procedure called the "relaxation method." Scripts were written to solve Laplace's equation on multidimensional unstructured and structured meshes. The applicability of using this method to solve Poisson's equation for electrostatic potentials in a dielectric continuum model is investigated in this paper. Mesh geometries and nearest neighbor amounts in relative directions and in quantity pose problems to compute the Laplacian at every node. Using weighting functions and adaptive mesh refinement can enhance interpolating field values at arbitrary points between mesh vertices. Properties of unstructured mesh in 3-dimensions show statistical Gaussian properties of nearest neighbor amounts, average nearest neighbors, areas of faces of tetrahedral, and edge lengths.

Particle Physics in a New Dimension: Web Development for "HiddenDimensions.org". *ARIANE LEE (University of Arizona, Tucson, AZ 85721) MICHAEL BARNETT (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

HiddenDimensions.org, a website currently in the development stage, is a site geared toward students and the general public who are interested in particle physics. The site focuses on the newest and most exciting areas of particle physics including string theory, mini black holes and gravitons. The main emphasis is on aspects of each field that may be explained with the idea of hidden dimensions. The basic content and format for the site was taken from a previously

created eight-page brochure that covers only the basics of each area of interest. On the website, these areas are being expanded and new content is being added. Many of the graphics from the original brochure are being animated into Flash movies that use both text and visual explanations to make the message clear and interesting. Putting animations on the website not only allows us to explain ideas through movies, but also gives a more interactive aspect to the site. Overall design for the website was created to be stylistically similar to that of the original brochure. Similar fonts were used and the title image was taken from the original artwork. A sidebar and navigation buttons were created to make each page as user friendly as possible. HiddenDimensions.org is still under development and will hopefully be completed by the end of this year. The site will continue to grow as content beyond that provided in the brochure is added.

Power Density Spectral Analysis as a Method of Compact Object Determination in X-ray Binary Systems.

JOHN LEE (Taylor University, Upland, IN 46989) **PABLO SAZ PARKINSON** (Stanford Linear Accelerator Center, Stanford, CA 94025). Mass determinations and X-ray energy spectral analyses are among the methods used to distinguish between the types of compact objects present in X-ray binary systems. We test a method of distinguishing between neutron stars and black holes proposed by Sunyaev and Revnivtsev where power density spectra are used, particularly in the 500-1000Hz range. Sunyaev and Revnivtsev found that only neutron stars appear to have significant power in this frequency range. We apply this criterion to 12 X-ray binary systems (six neutron stars and six black holes) using USA data and cannot reproduce Sunyaev and Revnivtsev's result. The reason for this discrepancy is most likely a USA instrumental effect which manifests itself as excess power in the frequency range of interest. Future work on correcting this problem should provide more accurate analyses that may yield a different result.

Analysis of the Characteristics of the Electron Cloud Build-Up in High Energy Particle Accelerators Using the Java Programming Language.

LAURA LOIACONO (Loyola University Chicago, Chicago, IL 60626) **KATHERINE HARKAY** (Argonne National Laboratory, Argonne, IL 60439). A phenomenon, known as the "Electron Cloud Effect", has become important for accelerator physicists to understand in an effort to increase the efficiency and quality of particle beams. A result of the photoelectric effect, the "electron cloud" is comprised of photo- and secondary electrons that can interfere with an electron or positron particle beam circulating in the storage chamber. At the Advanced Photon Source (APS) at Argonne National Laboratory, data have been collected on the characteristics of this electron cloud using detectors designed and constructed by researchers at the APS. The data show high densities of electrons comprising the cloud under specific conditions. One theory that suggests that this phenomenon can be explained by a resonant electromagnetic interaction between electrons in the cloud and the charged particle beam, known as "beam-induced multipacting", only partially accounts for the data. In an effort to fully explain the high densities of cloud electrons shown in the data, an "alternate resonance" theory was developed that suggests the secondary electrons play an important role in the resonant interactions. To determine validity of the latter theory, several computer programs that provide a quantitative analysis of the cloud-beam interactions were developed. By examining the energy imparted to the cloud electrons by the charged particle beam and their resulting motion, resonant beam-cloud interactions can be determined. Preliminary results suggest that an alternate resonance condition among secondary electrons exists in the storage ring at the APS for a variety of beam parameters.

Experimental Setup for Zircaloy Fuel Rod Cladding Experiments; Spike Oxidation Kinetics and Auto-ignition.

CASSIDY LUDLOW (Lafayette College, Easton, PA 18042) **KEN NATESAN** (Argonne National Laboratory, Argonne, IL 60439). With recent terrorist attacks, concern about the safety of the nuclear industry is understandable. Because of this, it is important to study the temperature rise, pressure buildup, and possible explosion of uncontrolled spent nuclear fuel in the United States. By simulating the conditions of high temperature (up to 1300 degrees Celsius) and high internal pressure (both from helium gas and expanding ceramic pellets), one can look at the changes that a Zircaloy nuclear fuel

cladding undergoes as it approaches burst conditions. This set of experiments, to be carried out in the future, will do just that.

Creating a Strong Electric Field in a High Vacuum.

LUKE LUGINBUHL (Illinois State University, Normal, IL 61790) **ELAINE SCHULTE** (Argonne National Laboratory, Argonne, IL 60439). As a part of an Electric Dipole Moment (EDM) measurement, a set of high voltage electrodes must be designed and tested. These electrodes (also called field plates) are a prototype of those to be used in a measurement of the atomic EDM of Radium-225 (225Ra). To reduce the amount of unwanted gas molecules, the electrodes are set up in the presence of a high vacuum system. There is a tendency under the conditions of high voltage, small gap length between the field plates, and low pressure to produce electric breakdown, which is an undesirable effect. Electric breakdown occurs when an arc of electricity jumps across the gap between the electrodes dissipating the stored energy in the electric field. The goal of this project is to setup up a strong electric field in a high vacuum system between the prototype field plates. The electric field needs to be extremely stable. Once this is set up without any malfunction, a new set of electric field plates must be designed or the original plates must be modified so the 225Ra can be introduced into the electric field and tested for an Electric Dipole Moment. The electric field was not set up in the given time period because of some unexpected delays. However, the vacuum system worked properly and obtained a pressure of 1.4×10^{-5} Torr. In conclusion, the experiment was successfully setup and is almost ready to establish the electric field between the electrodes.

Modeling Relativistic Muons in Electromagnetic Storage Rings via Object Oriented Techniques.

TOMASZ MALISIEWICZ (Rensselaer Polytechnic Institute, Troy, NY 12180) **YANNIS SEMERTZIDIS** (Brookhaven National Laboratory, Upton, NY 11973). The Muon g-2 Experiment at Brookhaven National Laboratory consists of the world's largest super-conducting magnet, which is used as a muon storage ring. Since the arrangement of magnetic and electric fields plays a critical role in the experiment, computer simulations can be very valuable for studying beam dynamics. By adhering to the tenets of object oriented programming, a highly flexible program was developed in C++ in order to study the effects of different electromagnetic ring configurations and muon initial conditions. The use of abstract base classes, inheritance, and polymorphism allowed the easy incorporation and testing of several different algorithms for solving the necessary differential equations. The program's results demonstrated the dependence of Coherent Betatron Oscillation (CBO) amplitude on the muon initial conditions and a dependence of CBO frequency on weak focusing field intensity. A study showed first order methods for solving differential equations inadequate for the simulation and the Runge-Kutta fourth order method as suitable for studying particle dynamics. The program showed Object Oriented Programming (OOP) to be an effective mechanism for analyzing different numerical algorithms and simulating particle dynamics.

Dielectric Optical Coating Damage During Ultrafast, Ultraviolet Lasing.

ANDREA MUNRO (University of Washington, Seattle, WA 98195) **MICHELLE SHINN** (Thomas Jefferson National Accelerator Facility, Newport News, VA 23606). There is no data currently available for the laser induced damage thresholds (LIDT) of dielectric coated mirrors for ultrafast, high pulse repetition frequency (PRF) lasers operating in the UV. This is a critical value to know for the UV-FEL upgrade. Calculations predict that the cavity mirrors will be subjected to a maximum fluence of 0.7 mJ/cm^2 . We constructed a laser damage test facility to mimic the UV-FEL intracavity conditions at 400 nm, in order to test high reflector (HR) mirrors from several vendors. To date, we damaged a $\text{SiO}_2/\text{Ta}_2\text{O}_5$ dielectric mirror that was coated by electron beam deposition. The coating was damaged at 0.135 mJ/cm^2 . Further research is required to determine how the LIDT varies based upon the dielectric coating material and the technique employed to apply it.

A DC Glow Discharge for a High School Classroom.

HENRIETTA ONUMAH (Oberlin College, Oberlin, OH 44074) **ANDREW POST-ZWICKER** (Princeton Plasma Physics Laboratory, Princeton, NJ 08543). The objective of the project is to create a safe, affordable, portable, computer interactive, and multifunctional DC glow discharge tube for use in a typical high school physics classroom. Our goal is to use this

device not only to capture and create interest in plasma physics but as a tool to engage students in an active exploration of a variety of physics topics. We present the design, operation and labs created with our discharge tube. We are creating a selection of labs ranging from current/voltage relationships to spectroscopy that can be done on our setup. We have evaluated the vacuum chamber material- glass vs. plastic, our electrode spacing- a fixed vs. variable, external electronics with an emphasis on the power supply, safety and ease of use. Our design is an accessible 6 inch long tube with an inner diameter of 2 inches, which attains low pressure of about 20- 40 mTorr.

Photoionization of Multiply Charged Fe³⁺. *OLGA OVCHINNIKOV (University of Tennessee - Knoxville, Knoxville, TN 37996) FRED SCHLACHTER (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

The photoionization of Fe³⁺ was studied for the first time using synchrotron radiation from the Advanced Light Source (ALS) and the merged-beams technique. Fe³⁺ ions were successfully produced using ferrocene in an electron cyclotron resonance ion source (ECR). The measured yield of Fe⁴⁺ photoions as a function of photon energy revealed the presence of resonances that correspond to excitation of autoionizing states. These resonances are superimposed upon the photoion yield produced by direct photoionization, which is a smooth, slowly decreasing function of energy. The spectra for the photoionization of Fe³⁺ will be analyzed and compared with theory. The data collected will also serve to test models for the propagation of light through ionized matter.

Ion Release Curves for Isotope Separation On-Line Targets. *DANIEL PETERSON (University of Notre Dame, Notre Dame, IN 46556) BRAHIM MUSTAPHA (Argonne National Laboratory, Argonne, IL 60439).*

When an isotope is created in an isotope separation on-line (ISOL) target, the time it takes to leave the target is given by the sum of the diffusion and effusion times. The effusion can only be given by a statistical distribution, but the diffusion process can be described by a known formula. A simple parameterization of the effusion time distribution generated by the GEANT-4 simulation of the Radioactive Ion Source Test (RIST) target at CERN was found. Combined with the analytical formula of the diffusion time distribution, the parameterization produced a complete analytical model for the release process. This allowed computerized statistical fits of release data to be performed, replacing the manual fits used in earlier studies. This analytical formula gave the expected statistically relevant fits, which in turn provided values for the release parameters such as the diffusion coefficient and the sticking time for the studied nuclei. These values can be used to predict the release of the same nuclei from different target geometries without building and testing them.

One-Meson-Exchange Interaction Between Two Nucleons.

MARTY PICKENS (Monmouth College, Monmouth, IL 61462) T. S. HARRY LEE (Argonne National Laboratory, Argonne, IL 60439). Photodisintegration is the name given to the reaction characterized by an equation. What the equation basically states is that, when a photon of some energy is shot into a deuteron nucleus, a proton and a neutron are then emitted from the deuteron. After this experiment was performed at Jefferson Lab, it was noticed that different numbers of protons and neutrons were scattered at different angles relative to the photon beam's target, the deuteron. The measurement of the discrepancy in the number of particles in a particular cross section in relation to the total number of particles is called the differential cross section. The ultimate goal of my research here at Argonne is to achieve an understanding of these resulting emissions of neutrons and protons and the elastic scattering involved between them after the photodisintegration process. With this data from Jefferson Lab containing these resulting differential cross sections and angles characteristic of different photon energies, my time will be spent developing and utilizing a Fortran program that will then fit this data to a particular function. It is my hope that this programmed function can then be used to determine the behavior of the scattered neutrons and protons by estimating the various differential cross sections and angles associated with different photon beam energies.

Application Development of Cathode Strip Chamber Production Database for the ATLAS Experiment. *ARAN SAKZENIAN (Richland College, Dallas, TX 75243) KETEVI A. ASSAMAGAN (Brookhaven National Laboratory, Upton, NY 11973).*

The ATLAS Experiment is a global initiative to develop a large subatomic particle detector. It is a massive effort demanding the expertise of approximately 2000 physicists worldwide. Brookhaven National Laboratory physicists, among other things, have been working on a special part of the ATLAS Detector called the Cathode Strip Chambers (CSC). The main task for this internship was to develop computer programs using several software applications that would give scientists and researchers web-access to a database application, which would house testing results for the CSC. An object-oriented language, LabVIEW, was used to create a program that would switch the existing data from previous tests from .dat extension to a new Access database table format. LabVIEW was also used to change existing testing programs into a format that would write the results in an Access database table automatically, no longer writing them in a .dat extension format, and automatically saving the front panel of the test that was run for future reference. Next, a Visual Basic application was developed to arrange the test results in a user-friendly format and provide some helpful features such as statistical tools and images for scientists and researchers to be able to analyze test results from the database. A web page was then constructed using Dream Weaver 3 software that contained a summary of the database application and a link to enable scientists and researchers to download it.

Spectral Analysis of the Black Hole Candidate 4U 1630-47. *RISHIK SAXENA (University of California at Berkeley, Berkeley, CA 94702) DEREK TOURNEAR (Stanford Linear Accelerator Center, Stanford, CA 94025).*

We performed spectral analysis on the 1999 X-ray outburst of the soft X-ray transient black hole candidate (BHC) 4U 1630-47, in order to learn about physical processes (such as changes in inner disk radius of the accretion disk) that manifest themselves as changes of state. This source goes through an outburst every 600 - 690 days, which is a very short time period compared with other transient X-ray sources. The overall shape of the outburst's light curve was very similar to that of the 1996 outburst, but noticeably different from that of the 1998 outburst. We fitted 47 observations of the outburst to a model consisting of a disk blackbody, inverse Comptonization power law, and Gaussian component, multiplied by an absorption constant and an overall normalization constant. We found that the BHC progressed from a low state to high, and then back to low during its outburst. This pattern is common to persistent sources, not transient sources. We also found that when the source is in the low state, the flux and hardness are anticorrelated, as is predicted by theory. However, when 4U 1630-47 is in the high state, it is unclear whether or not the flux and hardness are correlated as theory says they should be.

RF Coupling Schemes for the SNS Ion Source. *SONALI SHUKLA (University of Tennessee - Knoxville, Knoxville, TN 37916) ROBERT F. WELTON (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

The ion source for the Spallation Neutron Source (SNS), initially developed at LBNL, is under going continuing development at ORNL. It is a radio frequency (RF), multi-cusp, ion source. The extracted H-beam current from the source is limited by the amount of RF power which can be coupled into the source plasma through an antenna, generally ~1 mA of H- per 1 kW. Operating the RF supply (80 kW) at excessive power levels to achieve a given H- beam current not only shortens the lifetime of the RF supply but also accelerates the deterioration of other electronic components of the ion source, control system and the front end of the accelerator, significantly reducing the availability of the SNS. Since coupling changes with time, the plasma stability is subject to change, adversely affecting the H- generation and beam formation. It is therefore critical to achieve excellent matching between the RF generator and source plasma. In order to do so, Berkeley has developed two matching schemes: a low-loss capacitive network and a transformer-based network currently installed on the SNS front end. This work presents an experimental characterization of each system using spectroscopic methods to determine the relative plasma density and therefore the relative efficiency of plasma coupling. Both networks required significant modification from their original form to achieve stable operation at full duty factor. From an operational point of view, this work represents

the initial commissioning of the hot spare stand for the SNS ion source with plasma.

Automated RF Cavity Conditioning with EPICS for Spallation Neutron Source Linear Accelerators. ERIC SNOW (*University of California, Berkeley, Berkeley, CA 94720*) JOHN GALAMBOS (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

High-powered radio-frequency (RF) cavities are the basis for the Spallation Neutron Source's (SNS) linear accelerators. Three different types of linear accelerators, some of which consist of cavities powered by mega-watt klystrons, are to be commissioned by the SNS. High power cannot be immediately applied, however, as irregularities in materials and foreign particles inside the cavities will cause intense arcing, and may severely damage the accelerators. Power levels must be raised slowly while monitoring for sparking. Previously the operator has done this manually, but higher power levels may be achieved sooner when done under computer control. Sparking is detected using a calibrated pickup loop inside the cavity; an analog to digital converter will read the power level near the end of the RF pulse. If the acquired power level is low enough it is counted as a spark, as an electric breakdown will reduce the local field. SNS has chosen to use the Experimental Physics and Industrial Control System (EPICS), and the conditioning program is written as an EPICS Sequence program because of the ease in which it can generate finite state machines. The power ramping algorithm implemented is piecewise linear; the operator specifies the beginning power, two thresholds and a final power, as well as the rate of change for each of the three regions. When sparking reaches a critical level, RF power is immediately dropped, and the rate of change for the current leg is reduced by one-half. A simulator was written to provide sample input to the program.

Uncovering the Electrical Properties of Four Potential Superconductors through Construction of a New Cryogenic System and Associated LabVIEW Program. JENNY TOBIN (*Albion College, Albion, MI 49224*) DAVID K. CHRISTEN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Superconductivity has the ability to revolutionize the distribution of energy in the form of electrical power. The negligible resistance in superconductive materials makes them much more efficient than existent materials as carriers of electricity. Presently materials found to be superconductive do so at low temperatures (near the boiling temperature of liquid nitrogen, 77K). A cryocooler is a mechanical device with the ability to reach and maintain these low temperatures using compressed helium gas. In a cryocooler, superconductivity was measured on the sample through a four terminal reading of electrical resistance. This type of measurement, taken while cooling and warming, increases the accuracy for small values of current and voltage. LabVIEW (a graphical programming language) was used to develop a program to control the temperature, evaluate the amount of current forced through four potentially superconductive film samples and measure the voltage across each of the samples. These values were stored in LabVIEW and were used to calculate resistances that were then graphed against the sample temperature. The program was customized to provide a sufficient density of recorded values during the abrupt resistance decrease that occurs at the superconducting transition temperature, T_c , below which the resistance is zero. The plot also examined the direct relationship between resistance and temperature in the normal state above T_c . Materials tested in this manner include thin film samples of $YBa_2Cu_3O_x$ and $NdBa_2Cu_3O_x$, compounds synthesized on assorted substrates and composite $Bi_2Sr_2Ca_2Cu_2O_x/Ag$.

Building a Pulse Detector using the Frequency Resolved Optical Gating Technique. JOSE VALLIN (*San Jose State University, San Jose, CA 95192*) PAUL BOLTON (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

We show how to construct a diagnostic optical layout known as Frequency Resolved Optical Gating (FROG) for an infrared mode-locked laser by using the nonlinear effect known as second harmonic generation (SHG). In this paper, we explain the principle of operation and the theory upon which this diagnostic is based. Moreover, we described the procedure used to measure the duration and frequency components of a pulse. This process consists of calibrating the scales of a two-dimensional image, time delay vs. frequency, known as FROG spectrogram or FROG trace. This calibration of the time delay scale yields the correspondence between a pixel and time delay. Similarly,

the calibration of the frequency scale yields the correspondence between a pixel, and frequency.

Muon Trigger Upgrade for PHENIX. GREG VER STEEG (*Drake University, Des Moines, IA 50311*) MATTHIAS GROSS-PERDEKAMP (*Brookhaven National Laboratory, Upton, NY 11973*).

Experiments with high energy, polarized protons at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory will produce data allowing new insights into the spin structure of the proton. The parity violating nature of the electroweak force enables a direct measurement of the spin contribution of individual flavors of quarks and anti-quarks via the W production channel. To date, no such measurement has been made. The PHENIX detector at RHIC is capable of detecting muons from the decay of W bosons in the pseudo-rapidity range from 1.2 to 2.4. These muons, however, are obscured by soft muon production from hadron decays. For polarized proton collisions at the expected luminosity, the current muon trigger cannot sufficiently filter the desired, higher momentum muons (>10 GeV) from the muons in the background (~2 GeV). We studied three proposals for upgrading the PHENIX detector. First, we studied the use of a new hodoscope with which tracks through the magnetic field could be reconstructed in real time. Second, we investigated the addition of a threshold Cherenkov counter for distinguishing high momentum muons. Finally, we studied the utility of using a nosecone calorimeter to distinguish events based on topological differences. Simulation results studying feasibility and design considerations will be presented.

Characteristics of Neutron Imaging Devices. MICHAEL VIRDONE (*State University of New York at Buffalo, Buffalo, NY 14261*) GRAHAM C SMITH (*Brookhaven National Laboratory, Upton, NY 11973*).

This paper describes research work on position sensitive neutron detectors. It is essentially a continuation of research that the author carried out in the summer of 2001, under the ERULF program. Whereas last year the work involved general research with a new project, this year some specific characteristics have been investigated. These include application of the newly developed encoding electronics to existing planar detectors from BNL's neutron spectrometers, calculation of effective radii of curvature (of the 120° detector) as a function of neutron wavelength (a key parameter required for Los Alamos users of this detector), and quantitative measurements of a new UV exposure instrument used in the fabrication of neutron detector electrodes. The results from all these activities are of prime importance for the long-term participation of BNL's detector group in DOE's neutron user program.

Investigation of Energetic Electron Production by Ultraintense Laser Ionization of Highly Stripped Atoms.

PETER WEIR (*University of California - Berkeley, Berkeley, CA 94720*) NATHANIEL FISCH (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

It has recently been predicted that GeV electrons can be produced by the interaction of ultraintense lasers with highly charged ions. This acceleration process is investigated by numerically integrating the relativistic electron equations of motion in which the bound state of the electron is approximated as a classical Kelperian orbit. The ionization of an electron from 22-times ionized vanadium by a laser pulse of intensity 10^{21} W/cm² is considered as a specific case. An analytical approach to predicting electron energy distribution is presented.

Temperature Calculations for a Rotating Target Wheel Under Intense Beams for Super-Heavy Element Production. JENNIFER WELSH (*University of Illinois at Urbana-Champaign, Urbana, IL 61801*) JOHN P. GREENE (*Argonne National Laboratory, Argonne, IL 60439*).

Intense beams are needed in the production of the heaviest elements as a consequence of very small fusion cross sections. Thus, the targets used will have shortened lifetimes as the beam current is increased. When a tightly focused beam hits a stationary target of modest melting point and/or a high sputtering yield material, the target will eventually melt or be destroyed. Using a rotating target wheel can help to overcome target melting and adding a thin covering of a low sputtering rate material will help to protect the target. This allows for higher beam currents to be applied. Using a defocused or a "wobbled" beam can enhance target survival as well. The purpose of the calculations done for this work is to attempt to predict the safe range

of beam currents that produce a heat load below the melting point of the target material. Calculations of the target temperature after beam exposure will show the safe limits to which they may be exposed without being destroyed.

Photoelastic Modulation as Means of Polarimetry for the Rattlesnake Mountain Observatory. MICHAEL WHIPPLE (Salt Lake Community College, Salt Lake City, UT 84115) NORMAN C. ANHEIER (Pacific Northwest National Laboratory, Richland, WA 99352).

Polarimetry is a powerful tool used by astronomers to characterize light from celestial objects and infer their properties. The Rattlesnake Mountain Observatory intends include polarimetry in its study of the universe. A series of experiments were performed to understand how to collect and interpret polarimetry data obtained using a Photoelastic Modulator (PEM). Lasers, linear polarizers, and birefringent wave plates were used to produce light with known states of polarization. These polarization states were analyzed using a photodetector, oscilloscope, and the PEM. It was observed that each polarization state displayed its own distinctive waveform when analyzed through the PEM. Light was then generated with unknown states of polarity and analyzed. Repeated trials confirmed the accuracy of the PEM measurement technique.

Geometric Shape Conversion for Data Slicing in the ATLAS Experiment. WILLIAM WILTSIE (State University of New York at Alfred, Alfred, NY 14802) KEITH LALLY (Brookhaven National Laboratory, Upton, NY 11973).

The ATLAS experiment at the CERN laboratory in Geneva, Switzerland is a toroidal large hadron collider apparatus, which is scheduled to be completed in 2006. Scientists have run simulations using the capabilities of ATLAS and developed model output data in ROOT format. To evaluate this data, geometric shapes are needed to slice the data, which must be then exported to Open Inventor file format for further viewing and investigation. Data slicing using geometric shapes allows for more depth in the analysis of the data. The C/C++ programming language was used to manipulate the ROOT file of a particular geometric shape to produce an Open Inventor file in ROOT. The Open Inventor file was then imported to SceneViewer, which allowed for viewing and the ability to make initial corrections in the translated Open Inventor file. Upon identifying any mistakes, the ROOT coding was then changed. In the course of the programming, shapes such as a brick and a tube were successfully translated. Though this experiment is still in its infancy, it appears that translating shape files from ROOT to Open Inventor is a relatively smooth operation. This is extremely promising the future prospect of dissecting the ATLAS model data with translated shape files.

Simulated X-Ray Absorption Spectroscopy on the Water Dimer. AMY WUNG (University of California Berkeley, Berkeley, CA 94720) ANDERS NILSSON (Stanford Linear Accelerator Center, Stanford, CA 94025).

The ability of an individual H₂O molecule to form multiple hydrogen bonds with neighboring molecules makes it an ideal substance for the study of hydrogen bonding. X-ray absorption spectroscopy (XAS) can be used to study what intermolecular structures the hydrogen-bonded water molecules form. XAS excites core electrons from the oxygen 1s atomic orbital to an unoccupied orbital. The resulting absorption spectrum shows the energy levels of the unoccupied orbitals, which in turn is dependent on the intermolecular structure of the H₂O system. Previous studies using molecular dynamics computer simulations have concluded that the intermolecular structure of liquid water is a distorted tetrahedron. Yet x-ray absorption spectra show discrepancies between liquid water and ice Ih, which is already known to have a rigid tetrahedral structure. The research group, which is based in the University of Sweden in Stockholm and the Stanford Synchrotron Radiation Laboratory at the Stanford Linear Accelerator Center, has studied the possible presence of broken hydrogen bonds in the liquid water intermolecular structure to explain these deviations. Computer simulations are used to construct theoretical absorption spectra for models of liquid water including broken hydrogen bonds. Creating such models requires controlling variables. The simplest method of isolating individual variables, such as hydrogen bond length and angles, is to study the water dimer. Here, the water dimer is used to study how the absorption spectra change with the way the water molecules are positioned and oriented relative to each other.

SCIENCE POLICY

Undergraduate Research: Portfolio Assessment from the Classroom To A National Laboratory. GEORGE BISANZ (Oakland University, Rochester, MI 48309) ERIC P. LOEWEN (Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID 83415). This paper describes undergraduate research at US National Laboratory. The Idaho National Engineering and Environmental Laboratory has programs that bring undergraduate students to the laboratory to enhance their research experience. Methods capable of improving the quality of undergraduate engineering education are introduced. The methods and assessments discussed in this paper could help engineering programs receive accreditation from the Accreditation Board of Engineering and Technology (ABET), especially criterion 2, involving the dictation of educational objectives, measurable learning outcomes, assessment of student achievement, and feedback for improvement.

Potential Impacts of Efficiency Standards for Distribution Transformers. AMOZ ECKERSON (Milwaukee School of Engineering, Milwaukee, WI 53202) JOHN STOOPS (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

There is federal mandate to establish minimum operating efficiency standards for distribution transformers according to the Energy Policy Act of 1992. Approximately 50 million distribution transformers in the United States account for 61 terra-watt hours of electricity loss per year. Small improvements (0.1%) in average efficiencies can have a significant impact on long-term equipment cost savings, energy savings, and the environment. To predict these benefits, a model of future energy markets and scenarios was used. This model was a combination of economic predictions and engineering design optimization. The analyses used a range of inputs (as probability distributions) to produce future scenarios representing the potential implication of certain standard levels. The standard levels establish minimum operating efficiencies in the range of 98.6% and 99.5%. Multiple analyses were performed on different classifications of transformer design types. Costs and benefits were compared to determine the potential impacts of each standard level.

An Economic Evaluation of Desalination at Diablo Canyon Nuclear Power Plant. JASON KILSDONK (The University of Chicago, Chicago, IL 60637) JOE BRAUN (Argonne National Laboratory, Argonne, IL 60439).

Depletion of natural resources is a pressing issue that will affect much of the world's population in the near future. Supplies of fresh water are at extremely low levels in many countries, yet this impending crisis receives little media and government attention. Less than one percent of the world's total stock of water is fresh water, fit for human consumption. The coupling of diminishing fresh water supplies with an increasing population will force more people to live with inadequate amounts of water. A potential solution to this problem is desalination, a process transforming seawater into potable water. As part of a cooperative project to investigate the economics of nuclear desalination in the United States, Argonne was interested in a validation of the cost of supplying freshwater via the existing infrastructure at Diablo Canyon. By obtaining this estimate, Argonne would be able to determine how the cost of water produced through desalination compares to current local water supply costs. A second objective of this project involved manipulating the data from Diablo Canyon, and determining how water production costs change when various parameters are altered. Using the Desalination Economic Evaluation Program (DEEP), Argonne was able to verify Diablo Canyon's water production estimate, and suggest measures that could substantially lower these costs.

The Problems with the United States' National Missile Defense Program. STEPHEN LEMARBRE (Trinity College, Hartford, CT 06106) ROBIN ABRUZERE (Department of Energy (Headquarters), Washington, DC 20585).

The United States government is currently working towards the development of a National Missile Defense system that will protect the country from incoming Intercontinental Ballistic Missiles. The government, however, is spending billions of dollars on a program that is ultimately flawed and technically unfeasible. There are vast amounts of countermeasures capable of defeating a missile defense system

already accompanying Chinese and Russian ICBM's, and any "rogue nation" capable of building and/or purchasing ICBM's will have the ability to purchase and/or build the countermeasures to accompany those missiles. This missile defense system will go far beyond its projected date and cost. Whistleblowers have questioned the DOD on incorrectly relating its missile defense tests reports, and thus far the system has proved incapable at best. This report will examine the many problems with the proposed National Missile Defense System, and show why the United States should pursue other means of missile defense.

Recruiting a New Generation of Workers into NASA Related Fields. GREG MCILVAINE (*Vanderbilt University, Nashville, TN 37235*) MARY TOLER (*Department of Energy (Headquarters), Washington, DC 20585*).

The National Aeronautics and Space Administration (NASA) provides many benefits for our Nation, especially with technology, exploration, and economic progress. Presently, a current problem exists in the NASA workforce as the number of scientists and engineers age 60+ years old outnumber the under-30 workforce by 3 to 1, and close to 25 percent of NASA's S&E workforce is eligible to retire within the next five years. Thus, a significant increase in the number of new NASA recruits and expertise will be needed to continue important NASA activities in the future. However, despite NASA's incredible effort to recruit talent through outreach programs, educator workshops, university and private sector cooperation, and technology in the classroom, the number of individuals entering into aeronautical engineering and other NASA related fields is still declining. Thus, NASA must improve and expand their present strategies for recruitment, as well as establish new strategies for the future. One important strategy addressed in this paper is changing the cultural perspective of NASA and science and engineering related fields through the media. The media, one of the most influential elements in shaping American culture, can be used to transform the perspective of S&E related fields as being unpopular or difficult, into disciplines that are dynamic and exciting. Marketing strategies and how world events affect workforce trends will also be addressed.

The Access to Essential Medicines Problem: Options for Compulsory Licensed Exports Under the Doha Declaration. MICHAEL SEW HOY (*Rice University/University of Chicago Law School, Houston/Chicago, TX/IL 77005/60637*) ROBERT C. MARLAY (*Department of Energy (Headquarters), Washington, DC 20585*).

The developing world faces a serious access to essential medicines problem. Diseases that are treatable and/or manageable in the developed world, like HIV/AIDS, tuberculosis, malaria, and meningitis, have become public health crises in the developing world due to the high costs of pharmaceuticals. Many options have been presented to combat this problem, including the use of compulsory licenses for pharmaceuticals. However, under the World Trade Organization's TRIPS Agreement, there are serious deficiencies with the existing framework to effectively use such licenses. Even if a developing country could issue a compulsory license, they often lack the manufacturing capacity to actually produce the needed pharmaceuticals. The Doha Declaration at the 4th WTO Ministerial established a mandate to remedy this particular access problem: how to allow compulsory licensed exports into countries that lack manufacturing capacity. Three groups, the European Communities, the Developing Countries, and the United States, have proposed plans. Using TRIPS and the Doha Declaration as guides, the best plan to execute the Paragraph 6 mandate would be a modified TRIPS Article 30 interpretation of the Developing Countries' Plan. Such a plan would use the Article 30 interpretation as the legal mechanism to effect change, but would include some slight modifications from the Developing Countries' Plan to obtain broader support of all Members, while not sacrificing the effectiveness of the Plan. Effective use of the Plan could possibly go a long way to remedy the essential medicines problem.

Guide to Implementing Community Scale Wind Projects on Native American Reservations. TYSON UTT (*James Madison University, Harrisonburg, VA 22801*) TONY JIMENEZ (*National Renewable Energy Laboratory, Golden, CO 89401*).

The purpose of this paper is to provide a guide to implementing community scale wind projects on Native American reservations. Many tribes have an ideal situation for developing community sized wind projects on their reservations. The incentives include, but are not

limited to, abundant wind resources; sovereignty to control political and economic issues; federal support through development programs; and tribally owned community loads such as office buildings or casinos. Implementing a wind project to supplement the electricity demand of a tribally owned building presents some political and economic considerations unique to a tribal setting. The focus of this paper is how to implement a community wind project on tribal lands.

WASTE MANAGEMENT

Mesoscale Aerobic and Anaerobic Landfill Bioreactors. ALICIA WHITE (*James Madison University, Harrisonburg, VA 22807*) SHARON E. BORGLIN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Current regulations require the capping and lining of municipal solid waste landfills. While this is effective in controlling the release of harmful chemicals to the environment, this containment also limits biodegradation. Because landfills are becoming increasingly expensive to maintain it is necessary to find some way to further improve degradation rates while protecting the environment. To accelerate the biodegradation and stabilization of landfilled waste, both air injection and leachate recirculation were applied to mesoscale laboratory bioreactors filled with municipal solid waste. The purpose of this study was to compare the effect of aerobic and anaerobic treatment on the quality of the landfill leachate. The following conditions were compared: (a) aerobic treatment of waste with leachate recirculation, (b) anaerobic treatment of waste with leachate recirculation, and (c) waste with no air or water circulation. The anaerobic tank with leachate recirculation had leachate with higher levels of total phosphorous, total nitrogen, chemical oxygen demand, biochemical oxygen demand, total organic carbon, dissolved organic carbon, ammonia, metals and sulfides. The anaerobic tank also had leachate with higher concentrations of magnesium, manganese, iron, silicon, tin, calcium and potassium. The anaerobic tank began producing methane at day 20. The results demonstrate that aerobic treatment of landfills with leachate recirculation improves the quality of the leachate, the rate of stabilization, and amounts of greenhouse gases. (Spring 2002)

Modifications to the System Assessment Capability (SAC) Simulator to Account for the Variability of the Groundwater Table at Hanford due to Wastewater Disposal. SHARON KARLESKY (*Oregon State University, Corvallis, OR 97330*) WILLIAM E. NICHOLS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The Hanford site was used to produce plutonium for nuclear weapons. Since production cessation, the US Department of Energy has the mission of remediating the radioactive byproducts that were introduced into the environment during the production process. The System Assessment Capability (SAC) software simulator was developed to assess the flow and transport of contaminants throughout the Hanford complex and the impact these contaminants have had from 1944 (pre-production) until 3050 (1000 years postclosure). The initial SAC assessment represented a static groundwater table when calculating the amount of contaminant released from the vadose zone to the groundwater aquifer. In reality, the groundwater level varied over time depending primarily on the volume of wastewater discharged to the ground at disposal sites. In order to account for the effect this variability has on the predicted contaminant release to the aquifer, modifications were made to the base template files used as input by the SAC Vadose Zone Flow and Transport Module. When a SAC assessment was repeated with the modified templates, the release of technetium-99, tritium, uranium-238, and hexavalent chromium increased 13.47%, 5.20%, 4.24% and 1.84%, respectively. These results agree with expectations and reflect the shorter travel path within the vadose zone consistent with a higher groundwater table. Thus, the modifications will improve the prediction accuracy of future SAC assessments.

Mercury Characterization of Stockpile Soils. GENEANE WALSH (*The Richard Stockton College of New Jersey, Pomona, NJ 08240*) BIAYS BOWERMAN (*Brookhaven National Laboratory, Upton, NY 11973*).

Approximately 7000 yd³ of stockpiled soil remain at BNL after the remediation of the BNL Chemical Holes disposal pits. This soil must be analyzed for various hazardous materials, mainly mercury. The ASTD lab has been set up close to the stockpile soils to analyze for mercury

and other Resource Conservation and Recovery Act (RCRA) metals, so it can be determined how the soil will be disposed of. In the lab, the soil is analyzed for mercury using equipment and techniques such as an X-ray fluorescence spectrometer, (a bench Jordan Valley EX-6600 EDXRF (XRF)) and a Direct Mercury Analyzer. The XRF is the main piece of equipment the author used during this project and therefore the focus of the report. The equipment allows the researchers relatively quick analysis of the soils, so decisions can be made quickly about whether to segregate the soils and subsequently how to dispose of them. The project began in April and is scheduled to finish in September 2002. Up to this point, the analysis of the stockpiles of soil did not show levels above the EPA guidelines, and therefore the stockpiles will be shipped off as low-level waste.

Mesoscale Aerobic and Anaerobic Landfill Bioreactors. ALICIA WHITE (*James Madison University, Harrisonburg, VA 22801*)
SHARON E BORGLIN (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

Current regulations require the capping and lining of municipal solid waste landfills. While this is effective in controlling the release of harmful chemicals to the environment, this containment also limits biodegradation. Because landfills are becoming increasingly expensive to maintain it is necessary to find some way to further improve degradation rates while protecting the environment. To accelerate the biodegradation and stabilization of landfilled waste, both air injection and leachate recirculation were applied to mesoscale laboratory bioreactors filled with municipal solid waste. The purpose of this study was to compare the effect of anaerobic treatment on the quality of the landfill leachate, specifically with respect to metals. The following conditions were compared: aerobic treatment of waste with leachate recirculation and anaerobic treatment of waste with leachate recirculation. The anaerobic tank leachate had higher levels of total phosphorous, total nitrogen, chemical oxygen demand, biochemical oxygen demand, total organic carbon, dissolved organic carbon, ammonia, and sulfides. The anaerobic tank leachate also had order of magnitude higher concentrations of Mg, Mn, Fe, Si, Sn, Ca, and K. The results demonstrate that aerobic treatment of landfills with leachate recirculation improves the quality of the leachate increases the rate of stabilization and reduces the need for the leachate treatment. (Summer 2002)

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