

ABSTRACTS

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BIOLOGY

A Comparative Analysis for the Development of Polymerase Chain Reaction on Biochips. LAURIE RIESBECK (*University of Notre Dame, Notre Dame, IN 46556*) ALEX KUKHTIN (*Argonne National Laboratory, Argonne, IL 60439*).

Biochips, which consist of an array of probes attached to some surface, are the future of biological laboratory research. They are being used to revolutionize the pharmacology field, to detect hazardous microorganisms, and to understand life on a genomic level. PCR, or polymerase chain reaction, is a patented method for selectively cloning a segment of DNA. Using biochips to perform PCR will aid in quick and efficient identification of microorganisms that are possible bioterrorist threats, such as anthrax. In this experiment, PCR was performed on two biochips that contained the same reagents but consisted of different types of gel pads. To run PCR, each sector on the biochips was loaded with 1.2 mL of DNA, 3 mL of 10x buffer, 3 mL of 10x dNTP oligonucleotides, 3 mL of MgCl₂, 1.2 mL of forward primer HSNSpF1 and the same of the reverse primer HSNSpR1, 1.2 mL of tRNA, 0.6 mL of 100x BSA, 0.5 mL of Stoffel Fragment enzyme, and 15.1 mL of purified H₂O. When the PCR cycles were complete, a hybridization reaction was performed on the biochips in order to attach a fluorescent signal to the amplified DNA. Then hybridization cocktail that was loaded onto each sector of the biochips contained 10 mL of 3x buffer, 1.2 mL of tRNA, 0.3 mL of 100x BSA, 0.075 mL 1 pmole DNA k probe, and 18.42 mL of H₂O. Next the slides were analyzed by a fluorescent microscope that was equipped with a charged coupled device camera, which took an image of the biochip and quantified the amount of fluorescence present within the gel pads. Results indicate that there is still much work to do be done to improve the procedure for performing PCR on the biochips. On the first chip, it was evident that PCR did not work because no fluorescent signals were found after the biochip was hybridized. It is suspected that the primers did not behave as expected, causing the experiment to fail. The second chip failed because the gel pads became dislodged from their slide during the extremely hot conditions of PCR, so it could not be determined if PCR had been successful.

Analysis of Metabolic Pathways Using Dynamical Models. JIM ADDUCI (*Illinois Institute of Technology, Chicago, IL 60616*), MATHEW JOHNSON (*Ball State University, Muncie, IN 47304*), JOHN NARA-DZAY (*University of Maryland, Baltimore County, Baltimore, MD 21250*), and DMITRY KARPEEV (*Argonne National Laboratory, Argonne, IL 60439*).

The circadian rhythm is a common mechanism in cells that has remained mysterious despite extensive research on the subject. Several non-linear mathematical models were constructed and analyzed to investigate the following two hypothesis: the circadian rhythm contains self oscillations regulated primarily by the metabolic pathway, and that the redox state of thiols is an important circadian rhythm signaling mechanism. In order to produce fast transitions, justified theoretically and experimentally, we included positive feed back mechanisms in the pathway models. The glycolysis pathway (EMP), a common component of cell metabolism, was modeled and produced the desired fast transitions. An alternative to the EMP pathway is the pentose phosphate pathway (PPP), an example of which is found in *Synechocystis*. This pathway was similarly examined and yielded the desired oscillatory behavior. In addition, a generic mechanism found in EMP and PPP was considered in order to understand how genetic regulation of enzyme synthesis affects metabolic systems. For all parameter regimes examined, short enzyme influx modification produced a phase-shift in the oscillations dependent upon the impact the inhibition had on the active form of the enzyme. The magnitude of the phase-shift was directly related to the Michaelis-Menten constant of the inactive form of the enzyme, as well as the duration of the inhibition. Thus, chemical modification appeared to be a stabilization mechanism effectively minimizing the effects of enzyme influx. These results conform to our original hypotheses, although the effect of the addition of the other components of the metabolic pathway remains unknown.

Assessment and Analysis of Protein Complexes Across Archaea, Eukaryota, and Bacteria. RICHARD LUSK (*University of Chicago, Chicago, IL 60515*) NATALIA MALTSEV (*Argonne National Laboratory, Argonne, IL 60439*).

Analysis of protein subunit composition can answer questions in metabolic pathway research, genome analysis, and bioinformatics. To this end, we assembled a comprehensive database of manually filtered Swiss-prot subunit annotations for high-throughput analysis. Using this data, we assessed the distribution of enzyme complex sizes and types over the three domains, finding that eukaryotes tend toward smaller

[and more homogeneous] complexes, while archaea have larger and more complex complexes. Bacterial complexes are between those of eukaryota and archaea in both size and heterogeneity. We noted that multicellular eukaryotes show a higher proportion of large complexes and heteromers, and proposed that this is due to the higher rate of gene duplication among homomers in higher organisms. Our data show a large proportion of duplicate genes forming heteromers, supporting this hypothesis. The database is publicly available through both flat files and a web interface fully indexed and integrated with tools of special interest.

Deployment and Monitoring of Phytoremediation Techniques in Areas 317/319 of Argonne National Laboratory East. ASHLEY HARVEY (*Nebraska Wesleyan University, Lincoln, NE 68850*) M. CRISTINA NEGRI (*Argonne National Laboratory, Argonne, IL 60439*).

One of the most challenging environmental problems society faces is the process of decontaminating groundwater systems. There is a widespread problem of ground water contamination due to the abundant use of chemicals in industry, government, and households over the past century. Phytoremediation is a technology that uses plants in the environment to remove and/or degrade the contaminants in the soil and groundwater. The goal of this project is to use and monitor phytoremediation techniques to treat contaminated groundwater. In the 317/319 French Drain area of Argonne National Laboratory, groundwater and soil is contaminated with various Volatile Organic Compounds (VOCs), their degradation product trichloroacetic acid (TCAA), and the radioactive material, Tritium. Over 800 trees have been planted in this site and are being monitored and analyzed for traces of these chemicals. The following procedures are used; evapotranspiration monitoring for Tritium, soil monitoring for VOCs, tree sap flow determination, and gas chromatograph analyses of samples from the area. It was found that the trees planted in mixed soil have less contaminants present in their tissues than those planted in the non-mixed soil. This is due to the treatment of steam and iron that was applied to the soil previous to planting. This project is anticipated to be on going for the next five to ten years. The current focus of the project is collecting and analyzing samples through the growing season months (May-October) and then comparing the results as time progresses. The data that were collected are comparable to the results from previous years and it is expected that the levels of contaminants are being reduced. Unfortunately, due to lack of time, only a small amount of data was collected and analyzed. Also, because the project is still in a developing state it is difficult to draw accurate conclusions at the time.

Investigating Bead Array Hybridization using Total RNA versus Polymerase Chain Reaction Products for Viral Detection in Infected Plants. ROSHANDA RUFFIN (*North Carolina Agricultural and Technical State University, Greensboro, NC 27411*) DARRELL CHANDLER (*Argonne National Laboratory, Argonne, IL 60439*).

The Tomato Spotted Wilt Virus (TSWV) is a highly virulent tospovirus that has begun to affect plants that were originally non-susceptible to infection. Diagnostic analysis of gene expression is required in detecting infected plant tissue on specific genes. Recent developments in diagnostic analysis have shown that bead array technology has the potential to show greater multiplex detection than current techniques. Moreover, a rapid multiplexed assay for viral detection could facilitate early detection and prevention measures. We proposed to investigate bead array hybridization using total RNA and Polymerase Chain Reaction products as potential targets to detect TSWV. Initially, Plants were grown and inoculated with the viruses. After the plants exhibited viral symptoms, RNA was both isolated and extracted from viral infected and control plants. Using bioinformatics tools, primer pairs specific to the Nucleocapsid (N) gene of TSWV were selected to amplify capsid and replicase proteins. The selected primers permitted a Polymerase Chain Reaction (PCR) that prepared large amounts of nucleic acid. The PCR products and total RNA were then successfully labeled using the Alexa Fluor™ 532 labeling kit. Additionally, oligonucleotide probe sequences were covalently attached to individual sets of coupled microspheres. The final step in viral detection of TSWV requires additional optimization. We were unable to fully investigate the hybridizing of target nucleic acids to capture probes for analysis on the LiquiChip™ IS 100 flow cytometer. However, we are still investigating the hybridization of the nucleic acid to capture probes for viral detection on the flow cytometer. Ultimately, there was a significant increase in knowledge of bead array technology for detecting genetic mutations, and environmental microbial toxic threats in our environment.

Investigating the Application of the Argonne National Lab 3D Acrylamide Biochip for Detecting Tomato Spotted Wilt Virus in Infected Plants. OLAMIDE OLAYIWOLA (*North Carolina Agricultural and Technical State University, Greensboro, NC 27411*) DARRELL CHANDLER

(Argonne National Laboratory, Argonne, IL 60439).

Tomato Spotted Wilt Virus (TSWV) is one plant pathogen in a group of viruses referred to as Tospoviruses. It affects over 900 species of plants and is becoming increasingly important as a pathogen on a worldwide basis. To detect this specific virus, we investigated the application of the ANL acrylamide 3-D biochip (microchips covered by an array of tiny gel pads). This biochip is time-efficient, cost-effective and requires a relatively low consumption of reagents. Knowing the qualities that the ANL acrylamide 3-D biochip possesses, we hypothesized that if oligonucleotide probes derived from the TSWV nucleocapsid or replicase genes were immobilized on the hydrophobic acrylamide surface of the 3D biochip, then it could be used to detect the virus in infected plant tissue. Using the National Center for Biotechnology Information website, primers to amplify capsid and replicase target genes were selected. Complementary probes were synthesized and modified to have an amine group attached on the 3' end and then nanoprinted onto the biochip by the Quadrate 2 Robot. Target genes were amplified by RT-PCR and the concentration and integrity of the products were tested using a spectrophotometric assay and gel electrophoresis, respectively. The RT-PCR products were fragmented and labeled with lissamine rhodamine and hybridized to complementary probes that were immobilized on the biochip. The biochip was viewed using a fluorescence imager but no target DNA was detected. These results are preliminary and require further investigation before a conclusion can be drawn.

Production of a 200-probe Oligotide Microarray for Use in Bacterial Community Profiling. JULIE REBER (Duke University, Durham, NC 27708) MIROSLAVA PROTIC (Argonne National Laboratory, Argonne, IL 60439).

Monitoring bacterial community profiles is vital to the success of environmental bioremediation. Microarray biochips allow scientists to simultaneously test for the presence of up to 90 bacteria on one slide. Biochips consist of thousands of miniature test sites where bacterial DNA probes are hybridized with Cy-3 labeled 16-S RNA from environmental samples. Spots that have hybridized will fluoresce; they are then traced back to the original DNA samples, thus producing bacterial DNA-fingerprints that will identify organisms present in the environmental sample. This particular biochip is designed with 200 +0 and +10 bacterial DNA probes. The probes are diluted with print buffer and loaded into 384-well plates in a complex pattern that will produce adjacent rows of +0 and +10 probes in each well, with three replicate dots each. The GMS 417 Arrayer automates the production of microspots. Cy-5 in the print buffer fluoresces and allows the spots to be checked for quality control after printing. Scanning results show that precise conditions are imperative to microarray production; dust, water, and dirt produce noise that obscures the dots, and contact with light during printing fades the Cy-5 dye.

Software for Reading Metabolic Reconstruction into a Database Independent Object Model. MAURICE MCDOWELL (Governors State University, University Park, IL 60466-0975) SOON OK PARK (Argonne National Laboratory, Argonne, IL 60439).

The field of Systems Biology builds models of biological processes based upon experimental biological data. It is anticipated that these models will grow in size and complexity as we understand more about the dynamical aspects of these systems. These models presently use data that are spread over multiple databases. These databases represent similar data in dissimilar ways. Also, the structure of the databases change over time. Dissimilar database structures makes it difficult to construct models and the evolution of the databases over time result in wasted effort maintaining applications that use the data. A database-independent object model of the biological information can be used to insulate the application from these forces. In this project, we constructed software to read data from two dissimilar Oracle databases into a common object model. We first investigated technological choices for the project, comparing ODBC based database access with Python DBI based database access. We found the Python DBI to be a much simpler, but less capable, program interface but, since it met our needs, we chose Python and Python-DBI as the technological underpinnings for the project. We then implemented the object model in Python, wrote so-called 'factories' to read data from the two databases and convert the data into instantiations of the objects in the object model. We wrote test programs and, at the end of the project, connected the software to an independently produced application that was developed in terms of the object model. This application, a Python based Model Editor, will be improved in future work to allow construction of models from data in multiple databases.

Compositional Changes in Microdamaged Areas of Bisphosphonate Treated Dog Bones. MEGHAN RUPPEL (State University of New York at Stony Brook, Stony Brook NY 11794) LISA MILLER (Brookhaven National Laboratory, Upton, NY 11973).

There are an estimated 10 million people in the U.S. alone that have osteoporosis and another 34 million with low bone density, which puts them at risk for the disease. Bisphosphonates are a current class of drugs that are successful at treating osteoporosis, but it has been shown that high doses of these drugs increase microdamage in bone. This study used synchrotron infrared microspectroscopy to examine how bisphosphonates affect the chemical composition of bone in areas of microdamage. Bone samples (L3 vertebrae) were harvested from dogs that were treated with high doses (0.5 mg/kg/day) of oral risedronate (Actonel[®], Proctor and Gamble Pharmaceuticals, Inc.). Bones were fuschin-stained, embedded in methylmethacrylate and cut into 5 mm-thick sections. Areas containing microdamage were identified and infrared images were taken. Compositional analysis revealed that the level of mineralization in areas containing microcracks was the same as the surrounding undamaged areas, but collagen structure and carbonate content were different between the two areas. These results suggest that compositional differences in the microcrack areas may have affected the mechanical properties of the bone, making them more susceptible to cracking. Alternatively, the process of microcrack formation could cause a change in the composition of the surrounding areas of bone.

Deletion-Mutagenesis Analysis of the Interaction of the Human Adenovirus Proteinase with its 11-Amino Acid Cofactor pVlc. JEN-NIFER PEREK (University of Illinois at Urbana-Champaign, Champaign, IL 61820) WALTER F. MANGEL (Brookhaven National Laboratory, Upton, NY 11973).

The interaction of the human adenovirus proteinase (AVP) and AVP-DNA complexes with the 11-amino acid cofactor pVlc and deletion mutants of pVlc was characterized. The equilibrium dissociation constant (K_d) for the binding of pVlc to AVP was 2.2 mM. The binding of AVP to 12-mer single stranded DNA decreased the K_d for the binding of pVlc to AVP to 0.00578mM. The pVlc-AVP complex hydrolyzed the substrate with a Michaelis constant (K_m) of 2.28mM and a catalytic rate constant (k_{cat}) of 0.885 s⁻¹. In the presence of DNA, the K_m decreased less than 2-fold, and the k_{cat} increased 6-fold. To identify the amino acid residues in pVlc that are essential for the binding of pVlc to AVP and for the stimulation of AVP activity by pVlc, deletion mutagenesis was performed. Three residues, Lys6, Arg9, and Cys10, were the major determinants in the binding of pVlc to AVP, while Cys10 and Phe11 were the major determinants in stimulating AVP activity. While the binding of AVP to DNA increased enzyme activity in all of the mutants, it did not consistently increase or decrease AVP's ability to bind to the mutants.

Effects of Ultraviolet-A Radiation on Melanoma Induction in Xiphophorus Species. GAIL RICCIOTTI (Stony Brook University, Stony Brook, NY 11794) RICHARD B. SETLOW (Brookhaven National Laboratory, Upton, NY 11973).

Skin cancer is the most prevalent cancer in the United States, with melanoma being the most deadly form. Sunlight exposure is considered a contributing factor in its development. Sunlight is comprised of infrared, visible, and ultraviolet (UV) radiation. UV is divided into three ranges: UVA (320-400 nm), UVB (280-320 nm), and UVC (200-280 nm, absorbed by stratospheric ozone). UVA and UVB were found to damage DNA and cause immunosuppression. As damage from UV radiation accumulates, it causes cells to grow and divide abnormally resulting in cancer. When this occurs in a melanocyte, the resulting cancer is a melanoma. Small tropical fish of the genera Xiphophorus have been used as a model for research on melanomas. Learning just how UVA and UVB induce tumors in Xiphophorus might increase the understanding of melanoma induction in humans. To do this research female X. maculatus Jp163B were crossbred with the males of X. couchianus, a different species. The resulting backcross (interspecific hybrids) contained 25% pigmented fish. These individuals were used for this experiment because they contain only one tumor suppressor gene in contrast to normal fish which have two, and when exposed to UV they are more susceptible to developing tumors. A total of 360 fish were irradiated from above using the UVA light for 5 minutes at 600 J/m²/min. Of these fish, 94 developed heavy pigmentation and so were killed and preserved six months after irradiation. Histology was performed on 61 fish from five experimental groups. Tumors were found in 8 of the 61 fish. In the unirradiated controls, 2 of 31 fish developed tumors from the uncovered tank and 3 of 8 fish from the yellow cellophane covered tanks. There were 3 of 22 fish with tumors from the irradiated groups. There were more tumors found in the control than in the irradiated group. This experiment was inconsistent with the findings of previous experiments that UVA induces melanoma in Xiphophorus species.

Efficacy of Bacterial Degradation of Bituminous and Anthracite Coal. JEFFREY CHU (Stony Brook University, Stony Brook, NY 11790) MOW LIN (Brookhaven National Laboratory, Upton, NY 11973).

Bacteria are alleged to be a possible agent in a cleaner method of using coal than burning. The purpose of this experiment was to observe the efficacy of bacteria in degrading two common types of coal. Samples of bacteria were taken from some Virginia pine bark mulch and from Microbe-Lift Pond winterization treatment. Each sample was placed in a mineral medium with 2 grams of either anthracite (hard) or bituminous (soft) coal and allowed to progress for 22 days. The remaining coal in each setup was removed and weighed. Amounts of anthracite remaining exceeded those of bituminous coal after being degraded. Bacteria from the Microbe-Lift consumed more coal in both cases than those from the pine bark mulch. For the purposes of coal gasification, bacteria commonly found in mulch are less effective than ones used now for pond treatment are.

Identification and Distribution of Various Species of Adult Odonata at Brookhaven National Laboratory. MEGAN DYER (University of Rhode Island, Kingston, RI 02881) TIMOTHY M. GREEN (Brookhaven National Laboratory, Upton, NY 11973).

There are about 5,500 odonate species (dragonflies and damselflies) in the world, 164 of which can be found in the New York area. The purpose of this project was to identify and catalog the various species of dragonflies and damselflies inhabiting the wetland habitats of Brookhaven National Laboratory in Upton, New York. Specimens were collected in the field using a 15" white mesh insect net, a digital camera, chest waders, zip-lock bags, and a cooler full of ice. Specimens were identified in the lab using taxonomic keys, 20x field microscope, dissecting forceps, a refrigerator, and the Internet. There were a total of 25 species of odonates found to inhabit the ponds of the Lab, 18 dragonfly species and 7 species of damselfly. The data collected will be put together with other continuing research that is cataloging all species of flora and fauna found at Brookhaven National Laboratory.

Indirect Effects of Elevated Levels of CO₂ on Dark Respiration in Cottonwood. CHESSA GOSS (Community College of Rhode Island, Warwick, RI 02888) ANDREW LEAKEY (University of Illinois at Urbana-Champaign, Urbana, IL 61801) ALISTAIR ROGERS (Brookhaven National Laboratory, Upton, NY 11973).

At the current rate of increase, the pCO₂ atmospheric level will reach 70 Pa by the middle of this century (Prentice et al., 2001). To resolve the arguments surrounding indirect respiration, we examined the link between dark respiration and leaf chemical composition in *Populus deltoides* Barr (cottonwood) grown at elevated and ambient pCO₂ at the Biosphere II research center. We found a significant increase of R₂ at double (80 Pa) and triple (120 Pa) when compared to rates at ambient (40 Pa). On average this increase was 37% across both CO₂ levels. Increased starch, TNC, and protein contents observed at elevated pCO₂ were significantly correlated with R₂ rates, suggesting that as protein, carbohydrate content increases, rates of R₂ will also increase. If the same response were observed in other species, it would suggest that large increases in photosynthesis commonly observed in plants grown at elevated pCO₂ might be partially offset by increases in respiration.

Investigating the Data Quality Required for Determining the Structure of SeMet labeled ClpP for Input into SnB, a Phasing Program Based on the Direct Methods Technique. DAVID TAORMINA (Stony Brook University, Stony Brook, NY 11794) MARIA BEWLEY (Brookhaven National Laboratory, Upton, NY 11973).

X-ray crystallography is a powerful technique for determining the structure of proteins. In this, the scattering of X-rays by a protein crystal is measured. Additional information about the phase of the scattered ray is also required, but this cannot be measured directly. In the 1950s, Hauptman and Karle developed the direct-methods phasing technique that allowed the structures of small molecules to be determined. Increases in computing power and modern molecular biology techniques have allowed direct-methods to be applied to solving protein structures. However, a major limitation of this technique is that the signal-to-noise ratio is often small. For oligomeric proteins, one way of increasing this ratio would be to use the symmetry information, which is currently ignored. In this paper we will describe progress towards incorporating this information into the direct-methods package SnB (<http://www.hwi.buffalo.edu/SnB/SnBHome.htm>). The procedure and conditions used for protein crystallization, data collection, and our attempt to solve the structure using SnB will be described.

Lysozyme in Four Space Groups. ANNELIES RHODES (Dickinson College, Carlisle, PA 17013) VIVIAN STOJANOFF (Brookhaven National Laboratory, Upton, NY 11973).

The knowledge of the three-dimensional structure of proteins and biological molecules is key to the better understanding of the function of these molecules. The reproducible and controlled growth of large, well-formed, good quality crystals for X-ray diffraction has been

the bottleneck so far in the determination of the 3D structure of these molecules. One of the most common problems found by structural crystallographers is the non-isomorphism presented by some proteins during crystallization. Lysozyme, a 'bench mark' protein, is known to crystallize in at least four different space groups: tetragonal, orthorhombic, monoclinic, and trigonal. The purpose of this study is to determine similar growth conditions for all four of the different lysozyme space groups using the same protein concentration and growing all crystals at room temperature. Crystals were grown by the vapor diffusion method using the hanging drop technique. Lysozyme was screened separately for the four space groups and from these trays the best condition was chosen, from which another set of trays was prepared. Oil was also used with each of the conditions to better control the growth kinetics. In this experiment it was shown that lysozyme crystals can form in four different space groups at room temperature and with the same protein concentration even though different space groups may require different crystallization times.

Molecular Dynamics Simulation of Biomolecules Using Parallel Computers. ANSHUL SHAH (Harvard University, Cambridge, MA 02138) JAMES W. DAVENPORT (Brookhaven National Laboratory, Upton, NY 11973).

Molecular dynamics (MD) simulations can be conducted in an attempt to better understand biomolecular processes of interest, but computational power is a limiting factor in simulations involving proteins and other large molecules. Therefore, parallel computers are often used to distribute the computing load among many processors. In this study, the human adenovirus proteinase (AVP) is the model molecule for parallel MD simulations and energy minimizations using the AMBER force field. The experimental structure of AVP complexed with its cofactor pVlc provided the initial coordinates for simulations. MD and minimization were performed on both unsolvated and solvated systems, and both AVP-pVlc and isolated AVP (with pVlc coordinates deleted) were studied. Computation of van der Waals interactions between non-bonded atoms was cut off at a distance of 12 Å. Systems with water required greater simulation time in order to perform the same number of timesteps, but they scaled effectively to a greater number of processors. Root mean square (RMS) deviations from the experimental structure were found to be higher for isolated AVP than for AVP-pVlc after energy minimization, indicating that the natural state of uncomplexed AVP may differ from the complexed state. RMS deviations after MD simulation were comparable for both systems through 50 picoseconds, suggesting that more time steps may be required if a key structural change is to be seen in the isolated AVP structure. Comparison of the AVP simulation output to an experimental structure (currently unavailable) would allow for an evaluation of the MD method's effectiveness, but some support for the force field is already provided by small RMS deviations after minimization.

Preliminary Sequences for an MseI Burkholderia mallei Library. CAILIN WILKE (Cornell University, Ithaca, NY 14853) JOHN J. DUNN (Brookhaven National Laboratory, Upton, NY 11973).

The microorganism *Burkholderia mallei* (Glanders) is of interest to the U.S. Government because of its potential as a biological threat. The purpose of this experiment was to sequence part of the *B. mallei* genome. DNA from strain #23344 (China 7) of *B. mallei* was cut with the restriction enzyme MseI (T/TAA) and ligated into NdeI-cut (CA/TATG) pGEM5 vector. 5mL of the ligation was electroporated into ~50mL TOP 10 Electrocompetent cells using an Electro Cell Manipulator 600 (BTX). The electroporated cells were plated onto 100mg/mL Carbenicillin S. Gal (Sigma) plates with color selection. Sixteen potential positive clones were picked and grown up in 5mL 2xYT media w/Ampicillin (40mg/mL). The plasmid DNA was isolated using Qiagen's QiaWell Strip protocol (Qiagen), and the resultant DNA was sequenced using Amersham chemistry (Amersham Biosciences) on an ABI Prism 377 DNA Sequencer (Applied Biosystems). Three contiguous sequences were formed and edited using Sequencher 4.1 (Gene Codes Corporation), and two of these are perfect matches to parts of TIGR's (The Institute for Genomic Research) draft sequence of *B. mallei*. Analysis of these two contigs, with the Glimmer Program Suite (TIGR) shows that it is statistically unlikely that either sequence contains a protein gene, ORF, or a part thereof. However, a BLAST query showed that Contig. 0002 does contain part of the 16S rRNA gene, which is important for structure and function of the ribosome. Further studies will be conducted to determine the locations of methyl-CpG dinucleotides in the *B. mallei* (China 7, ATCC 23344) genome, and these results will be compared to those of other *B. mallei* strains.

Purification and Crystallization of ZitB, a Zinc Transporter from Escherichia coli. KATHERINE KAO (Stony Brook University, Stony Brook, NY 11790) DAXIONG FU (Brookhaven National Laboratory, Upton, NY 11973).

Cellular zinc homeostasis is essential to human health. Zinc transporters move zinc ion into and out of cells to maintain cellular zinc concentrations in a narrow range. Several membrane proteins have been shown to facilitate transmembrane fluxes of zinc ions, however, structures of zinc transporters are unknown. This work is to express, purify and crystallize a Zinc transporter, ZitB for crystallographic studies. ZitB was over-expressed as a His-tagged membrane protein using a pET15b expression vector hosted in *E. coli* BL21 cells. Purification of ZitB was achieved by preparation of ZitB-containing membrane vesicles, followed by detergent extraction, and completed with Ni-NTA metal affinity and size exclusion chromatography. The molecular identity of the purified ZitB was confirmed by mass spectrometry, showing an expected molecular weight of 35.2kDa. Crystallization trials of ZitB were conducted at 19.4°C using a series of low molecular weight PEGs as precipitants. Micro-crystals were grown in 25% PEG 1K, whereas only amorphous precipitations were observed in PEG 400 and 600. In conclusion, this work yielded highly purified ZitB protein preparation and defined an initial crystallization condition for ZitB.

Rodent Paradigm of Alcoholism: A Novel Dopamine D3 Receptor Antagonist Attenuates Alcohol Self-Administration in Ethanol-Preferring and Non-Preferring Rats. JOHN KATANA (*Wheaton College, Wheaton, IL 60187*) PANAYOTIS K. THANOS (*Brookhaven National Laboratory, Upton, NY 11973*).

The dopaminergic neurochemical pathway governs various neurological and psychiatric disorders, and is implicated in mediating addiction. Studies relating the dopamine D2 family of receptors to alcoholism and drug addiction have promulgated investigation as to the specific biochemical mechanisms involved. In the present study we examined the effects of acute antagonism of the D2-like D3 receptor on ethanol self-administration by alcohol-preferring P and non-preferring NP rats. We employed a two-bottle operant paradigm to monitor drinking behavior subsequent treatment with 3, 10, and 30 mg/kg SB-2770110-A, a novel selective D3 receptor antagonist. We report statistically significant efficacy of the D3 antagonist for P rats at the 10 and 30 mg/kg doses, in terms of percent ethanol preference and ethanol intake, and the 30 mg/kg dose, in terms of ethanol total lick responses; and for NP rats at the 30 mg/kg dose, in terms of ethanol intake and ethanol total lick responses. Furthermore, we report minimal extrapyramidal side effects, as indicated by stable lick response-volume ratios and lick response time distributions. Therefore, SB-2770110-A exhibits potential application as a therapy for human alcoholism, as well as neurological and psychiatric disorders.

Study of Ultraviolet-A and Ultraviolet-B Induced Killing of Melanoma Fibroblasts with or without Melanin. CYNTHIA ADDISON (*Edison Community College, Piqua, OH 45356*) RICHARD SETLOW (*Brookhaven National Laboratory, Upton, NY 11973*).

In the past 200 years, melanoma has dramatically risen in occurrence, with a lifetime risk of 1 in 90 in the United States. Absorption of ultraviolet light by DNA causes damage that, if not repaired, can become mutations that induce skin cancer [1]. Individuals with a genetic disease, Xeroderma pigmentosum, are sensitive to sunlight induced melanoma because of a defect in nucleotide excision repair of DNA [1]. The hypothesis is that in a study of cells exposed to different amounts of UV, in the UVB range, the survival rate of cells with high and low amounts of melanin will be about the same because both have the same principle absorber, DNA. In contrast, exposures in the UVA range, more cells are expected to survive with lower amounts of melanin when compared to higher amounts because melanin may act as a photosensitizer and react with DNA. Since UVA reaches the melanocytes, the proposed sensitization may be the explanation of the link between albino's, lacking melanin, having a very low occurrence of melanomas. Cells with and without melanin were exposed to different amounts of UVA or UVB, incubated for 14 days and colonies originating from single cells were counted. While not enough data were collected to form a firm conclusion, this experiment did show that cells containing melanin had a lower survival than ones without melanin after exposure to UVA. A second experiment was performed, but the 14 day waiting period is not over.

The Synthesis of Anhydrotrypsin: A Trypsin Still Shot. DONNA LEE (*University of California, Berkeley, Berkeley, CA 94720*) WALTER MANGEL (*Brookhaven National Laboratory, Upton, NY 11973*).

Trypsin, a digestive enzyme which hydrolyzes peptide and ester bonds, is a classic model of a serine protease. Of the most prevalent proteolytic enzymes, serine proteases utilize a serine residue in their active site to cleave peptide bonds. Previous studies have structurally characterized the later stages of hydrolysis, but the initial step of the reaction, substrate binding, remains elusive. Because of the tendency to rapidly progress beyond substrate binding, it is not feasible to obtain a static sample of trypsin bound to substrate pre-cleavage. However, it has

been shown that conversion of the active site serine to dehydroalanine to form the trypsin derivative, anhydrotrypsin, renders the protein enzymically inert but retains the ability to form stoichiometric complexes. In this study, we strived to synthesize and isolate this structurally intact yet inactive form of trypsin for the future purpose of protein crystallization of the anhydrotrypsin-substrate binding complex. With this end in mind, according modifications to the Ako et al. method were followed. Treatment with phenyl methyl sulfonyl fluoride (PMSF) as measured by the nitro phenyl guanidino benzoate assay rendered trypsin only 33% active. Thus, the potential formation of PMS-trypsin remained at 67%. Following base treatment and the addition of tosyl lysyl chloromethyl ketone, an irreversible inhibitor of active trypsin, separation was achieved by a soybean trypsin inhibitor (SBTI) affinity column. The separation profile revealed a relatively small nonspecific flow thru peak and a large specific elution peak. Because binding species alone would elute through the SBTI column, a sharp specific peak suggests that one species of binding intact trypsin was isolated from the separation. The appearance of multiple protein fragments upon SDS-page gel fractionation seemed to contradict this conclusion. However, removal of the reducing agent, resulted in two bands, an intense high molecular weight band, and a minor lower weight band. This indicates that the minor band was probably 'knicked' trypsin, trypsin with a cleaved bond with preserved conformation and ability to bind. The reduction of sulfur results in dissociation of the trypsin conformation whereas an unbroken disulfide bond alone retains the continuity of the protein. The formation of enzymically inactive, binding apt, and largely homogeneous anhydrotrypsin leaves the possibility of crystallization a promising prospect for further studies.

Tiger Salamander (*Ambystoma tigrinum tigrinum*) Emergence in Natural and Man-Made Ponds. KRISTINE HOFFMANN (*UMass, Amherst, MA 01003*) JEREMY FEINBERG (*Brookhaven National Laboratory, Upton, NY 11973*).

Although listed as Endangered in the state of New York, the eastern tiger salamander (*Ambystoma tigrinum tigrinum*) is abundant at Brookhaven National Laboratory. The purpose of this study was to compare the emergence of metamorphic salamanders from man-made and natural wetlands in order to develop better management strategies for the species. Drift fence arrays with pitfall traps were installed around two vernal pools, one man-made and one natural. Fences were checked in the morning and metamorphs were measured and released. Emergence from the man-made pond began 17 days before that of the natural pond. There is evidence that the larvae in the man-made pond are stressed due to overcrowding. Data from these ponds continues to be collected for further study.

Two-dimensional Crystallization of PapC, a Bacterial Pilin Exporting Outer Membrane Protein. DANIELLE THIBAUT (*Southampton College, Southampton, NH 11968*) HUILIN LI (*Brookhaven National Laboratory, Upton, NY 11973*).

PapC is a protein found in the outer membrane of bacteria. It acts as a transport channel in a pathway that allows bacteria to become infectious. Elucidating the structure of this protein can ultimately lead to further understanding of the methods through which this protein operates and to improved therapeutics. Two-dimensional crystallization provides an effective way to examine the structure of proteins. There are a variety of procedures that can be used to crystallize membrane proteins. In this study, PapC was slowly reconstituted into lipid bilayers through dialysis, allowing the protein to form crystals in its native environment. Although, this was a straightforward process, it was first necessary to determine the optimal conditions for crystal formation. Three different lipids were tested, DMPC, DOPC, and *E. coli* polar lipid extract, at 4°C or 25°C. In addition, many lipid to protein ratios (LPR) were examined. The crystals were analyzed by transmission electron microscopy. Crystal lattices were viewed at several different angles and photographed. It was concluded that the most favorable conditions for PapC crystal growth were in *E. coli* polar lipid extract dissolved in OG at 4°C, with an LPR of 1:1. The negative film images have been digitized with a high resolution scanner and will be processed by computer with Medical Research Council (MRC) image processing software – Image2000, which uses the range of angled views for each lattice to reconstruct the three-dimensional structure of PapC from a series of projections.

Variations in Carbohydrate Content of Glycine Max Grown Under Elevated CO₂ and Ozone Levels. LISA KISTLER (*Middlebury College, Middlebury, VT 05753*) ALISTAIR ROGERS (*Brookhaven National Laboratory, Upton, NY 11973*).

Plants grown under elevated carbon dioxide levels experience an accumulation of foliar carbohydrate content and a reduced photosynthetic capacity though it is thought that sink source balances alter this acclimation. Existing literature shows large variability in the effects of elevated CO₂ on plants demonstrating the need for tests to be conducted in a

natural environment. We used Free Air gas Concentration Enrichment technology to grow Glycine max (soybean) under ambient CO₂ and ozone levels, elevated CO₂ levels, and elevated ozone levels in a field. First fully unfolded trifoliolate leaves were cut from the plants at six different sampling periods over the growing season and analyzed for ethanol soluble carbohydrates, starch, total nonstructural carbohydrates (TNC), glucose, fructose, and sucrose. Plants of determinate and indeterminate cultivars were also grown and analyzed. We found a statistically significant increase at P=0.05 in foliar carbohydrate accumulation for plants grown under increased CO₂ that was highest during low reproductive activity and disappeared while plants were at the height of seed formation. Determinate plants showed larger carbohydrate accumulation in elevated CO₂ than indeterminate varieties. Varying sink capacities led to the excess carbohydrate accumulation experienced under elevated CO₂ where plants with low sinks showed a greater accumulation while plants with strong sinks showed little or no excess accumulation compared to ambient CO₂ levels. No significant difference was found between elevated and ambient ozone levels in carbohydrate content.

Importance of Violets for Meadow Fritillaries: A Study of a Butterfly and Its Habitat. KAMOLTORN KANGVANVONGSA (*University of Illinois at Chicago, Chicago, IL 60625*) TOM PETERSON (*Fermi National Accelerator Laboratory, Batavia, IL 60510*).

Meadow Fritillaries are relatively rare in northeastern Illinois but are abundant at Fermi National Accelerator Laboratory in Batavia, IL (40 miles west of Chicago). Previous observations from butterfly monitors at the lab suggested that they are strongly associated with fairly dense patches of violets. The purpose of this study was to characterize the Meadow Fritillary habitat at Fermilab and to gain greater knowledge of the relationship between this butterfly and violets, the caterpillar host plant. We also took a closer look at the influences of the neighboring vegetation on the Meadow Fritillary and the violets. The study was done by estimating the violet densities, and correlating the results with the densities of the Meadow Fritillary. The violet densities were measured by randomly sampling thirty-five one-meter squares within the 100-square-meter quadrat. Butterfly counting was done using two methods, standing and transect. The observations took place at four locations at Fermilab where the Meadow Fritillaries were abundant in the past two years and at one control plot with no violets. Prior to each observation, the date, time, temperature, weather conditions, and wind speed were recorded. The densities of violets were calculated as the number of violets per square meter, and compared to the average number of Meadow Fritillaries observed per day. The data indicated a positive correlation between the density of violets and the number of meadow fritillaries present. The effects of the weather, surrounding plants and the conditions of the neighboring vegetation on the Meadow Fritillary populations were minimal compared to the effect of the violet density.

Characterization of an Unknown Strain of *Paenibacillus glycanilyticus* Isolated from an Acidic Radionuclide-Contaminated Aquifer. CEDRICK WHITAKER (*Jackson State University, Jackson, MS 39203*) DAVID E. CUMMINGS (*Idaho National Engineering & Environmental Laboratory, Idaho Falls, ID 83415*).

Microbially mediated reduction and immobilization of contaminants plays a major role in bioremediation of large contamination sites such as the DOE Oak Ridge Reservation in Tennessee. Understanding the microbial diversity of such sites is the first important step in bioremediation. The focus of this research was strain A1 from a contaminated soil sample obtained at Oak Ridge Reservation and isolated by Alicia Olson at the Idaho National Engineering and Environmental Laboratory (INEEL). Following DNA extraction, the 16S rRNA gene was amplified, purified and sent to Washington State University where it was sequenced. The partial gene sequence was 99% (544/545) similar to *Paenibacillus glycanilyticus* strain DS-1 (AB042938). Our isolate, *Paenibacillus glycanilyticus* strain A1, was cultured in TSB medium in which it has an optimal growth temperature of 30°C with a range of 28-37°C, subdividing it as a mesophile. Its morphology is a *bacillus*, i.e., rod-shaped, with a Gram-positive cell wall. Although the contaminated well from which this strain came was at pH 4, A1 did not grow at pH 4, but had a pH optimum of 6-8. To discover the optimal carbon source for cell growth, strain A1 was incubated in a defined minimal medium with the following electron donors: lactate, glucose, glycerol, starch, or acetate. Acetate proved to be the best carbon source, supporting the most rapid growth and highest final cell densities. This culture of *Paenibacillus glycanilyticus* strain A1 may be one of the possible novel species that can immobilize contaminants such as uranium or technetium; in which case, adding *Paenibacillus glycanilyticus* strain A1 and acetate to a contaminated site could begin the regimen of bioremediation. Before this conclusion can be validated, further research such as determining the

optimal pH for growth, and which electron acceptors (i.e., contaminants) this organism may reduce.

A Study of potential Toxicity in Isolates of *Stachybotrys* species Obtained from the Chernobyl Exclusion Zone. OLIVER ROJAS (*Houston Community College - Northeast College, Houston, TX 77022*) GARY ANDERSEN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Stachybotrys chartarum, "the toxic mold" as it is referred to in the news, has gained a large amount of notoriety as an apparent producer of mycotoxins, chemicals that may be harmful to living organisms. Several isolates of *Stachybotrys* species from the Chernobyl Exclusion Zone were studied in an attempt to determine the presence of the Tri5 gene, which codes for Trichodiene synthase, an enzyme required for the synthesis of trichothecene, believed to be toxic to humans. Using custom made primers designed to amplify the Tri5 gene, DNA extracts from the isolates were subjected to PCR to determine if the isolates would test positive for the gene. Of the ten isolates, four showed enough evidence to deduce that they harbored the Tri5 gene. Another two isolates had faint bands at the correct molecular weight implicating the presence of the Tri5 gene. Test with alternate primers or modified PCR conditions will be needed to confirm the toxicity of these isolates.

Biological Assay of Rotenone Derivative's Inhibitory Activity to Complex I (NADH:Ubiquinone Oxidoreductase) of Electron Transport Chain in Mitochondria. EIGO SHIMIZU (*Seattle Community College, Seattle, WA 98119*) JAMES P. O'NEIL (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Rotenone is a well-known chemical with insecticidal, acaricidal, and piscicidal properties and can be obtained from the root of several tropical and subtropical plant species belonging to the genus *Lonchocarpus* or *Derris*. *Derris* root has long been used in South America as a fish poison to paralyze fishes and cause them to surface. Recently it has been used for insect control in the home garden, for lice and tick control on pets, and for fish eradication as part of water body management. It is known that at the molecular level rotenone binds to and inhibits NADH:ubiquinone oxidoreductase (Complex I) in electron transport chain in mitochondria, which are uniformly distributed in a relatively high concentration in the heart, the liver, and the brain. Considering the fact that rotenone binds to Complex I in mitochondria, which are found in a relatively high concentration in certain organs, rotenone could be considered a good radiotracer in Positron Emission Tomography (PET) and Single Photon Emission Computed Tomography (SPECT). Also it is important to note that the mass required for rotenone to bind to Complex I and be a PET/SPECT tracer is so small that rotenone would not make any significant interference with mitochondrial function. Recently we have synthesized several novel rotenone derivatives that could be candidates for radioactive tracer to diagnosis Parkinson's disease and certain organ defects. In this research, we study the inhibition activity of rotenone derivatives to NADH:ubiquinone oxidoreductase by measuring the rate of NADH oxidation by the enzyme inhibited by rotenone derivatives.

Building a Protein Binding Site Database for the Berkeley Drosophila Genome Project. NICHOLAS BLANCHARD (*California State University, Fresno, Fresno, CA 93740*) CASEY BERGMAN & SUSAN CELNIKER (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Genomic sequencing provides genetics with a context. Research that was previously unrelated is now part of a greater understanding of an organism. Laboratory research, however, remains somewhat segregated. Scientists are studying many different regions of the genome with limited knowledge of other ongoing projects. The consolidation of varied projects into organized and managed resources becomes necessary as science seeks a more complete view of an organism's genetic blueprint. Among the system-wide areas of study are the interactions of cis-regulatory modules. Researchers at the Berkeley Drosophila Genome Project have entered DNaseI protection assay data from numerous projects studying the role of protein binding sites in the regulatory system of *Drosophila*. Two programs, designed in-house, were used to place sequence within the context of the genome and specify binding factors in regulatory regions. The database could potentially benefit the fields of gene regulation, evolutionary studies, and medicine. Geneticists will be able to search for computational patterns of protein binding, traits of binding specificity, and shared genetic information between species.

Cell Wall Surface Layer Prediction through Chemical Extraction. RYAN HAMBLETON (*Brigham Young University, Provo, UT 84602*) TAMAS TOROK (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

In an attempt to develop a low-cost protocol that predicts the existence

of an S-layer in diverse strains of Bacilli, we compared multiple chemical S-layer extraction techniques on whole cells of *Bacillus licheniformis* and *Bacillus amyloliquefaciens*. The chemical agents used consisted of denaturants and salts at various concentrations and pH. With regards to denaturants, it was noted that an acidic solution of guanidine and a somewhat basic solution of urea were most successful in removing the S-layer. SDS-PAGE analysis was used to visualize extracted proteins allowing for the accumulation of circumstantial evidence that suggests the existence of an S-layer on *B. licheniformis*. However, our results for *B. amyloliquefaciens* were inconclusive, since these cells lysed under the extraction conditions resulting in a mixture of extracted, potential S-layer proteins with other cell proteins.

Domain Analysis of Two DNA Repair Proteins: CSB and MDC1.

CHRISTOPHER VU (University of Houston, Houston, TX 77204) **JILL FUSS, SUSAN TSUTAKAWA, AND PRISCILLA COOPER** (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). Human DNA is being repeatedly damaged by radiation and normal cellular metabolism creating lesions. If left unrepaired, this damage can lead to a loss of genomic integrity. Therefore, the human body has evolved multiple cascades of responses dependent upon the type lesion to repair this damage. The Cockayne Syndrome B protein (CSB) plays an essential role in the recognition of a stalled RNA polymerase II during Transcription Coupled Repair. MDC1 (Mediator of DNA Damage Checkpoint 1) is responsible for the recruitment of several proteins in order to induce repair of double-strand breaks. To begin to understand the exact mechanisms of CSB and MDC1 interactions with other proteins, a "divide-and-conquer" approach was taken. Six domains of CSB were amplified by PCR (Polymerase Chain Reaction) in two separate reactions: one reaction amplified the domain alone and the other reaction added a carboxy-terminal histidine tag to accelerate future purification. The PCR products were then subcloned into an expression vector that added an amino-terminal Glutathione S-Transferase (GST) fusion protein that will be used for purification and then removed by protease cleavage. First, the PCR products were subcloned into a Topo cloning vector that uses the topoisomerase enzyme to insert PCR products into the vector with high efficiency. Out of a possible 12 Topo constructs, ten were completed, one cloning attempt was unsuccessful, and one construct is pending confirmation. The Topo constructs were then digested using the restriction enzymes BamHI and XhoI, and the CSB domain sequences were ligated into an expression vector, pGEX-6P-1. One expression construct, the Acid-Nucleotide Binding Site (NTB) His tag construct, was completed and five other constructs are still in progress. These constructs will be used for expression of the separate domains of CSB to determine their interaction mechanisms with other TCR proteins such as XPG. GST-fusions of three MDC1 domains that were overexpressed in *E. coli* were purified from other cellular contents by GSTrap 1 ml columns for preliminary immunoprecipitation (IP) experiments. The helical domain, the repeats 1-7, and the C-terminus of MDC1 as well as the GST protein alone were eluted from GSTrap columns and transferred to a PBS solution by dialysis. Preliminary IP experiments were initiated but further studies are needed to modify the IP conditions to minimize non-specific interaction of the domains with the precipitation resin.

Exploring *Stachybotrys* Species from Chernobyl Exclusion Zone (CEZ) by Polymerase Chain Reaction using the IT51 and IT41 Primers.

SHANTA THOMAS (Houston Community College, Houston, TX 77022) **GARY ANDERSEN** (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). The Internal Transcribed Space regions in ribosomal DNA are variable regions that are flanked and spaced by highly conserved sequences of coding ribosomal genes. Regions of the ITS are more conserved within species than between species, making it a suitable marker for species identification. In this study PCR was used to amplify the ITS regions of ten *Stachybotrys* species isolates from the Chernobyl Exclusion Zone using primers IT51 and IT41. Seven of the ten isolates were successfully amplified; automated fluorescent sequencing will be done to analyze the nucleotides from the amplified regions.

Expression of p53 and p63 in Irradiated Differentiating Human Lens Cells.

MARCUS NEWMAN (Merced College, Merced, CA 95348) **ELEANOR BLAKELY** (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). p63 is a member of the p53/p63/p73 family of genes, located on the long arm of chromosome 3 (3q27-28). While p53 is primarily a tumor suppressor gene, the structurally similar p63 plays alternative physiological roles within the cell. p63 is critical for epithelial stem cell renewal and epithelial homeostasis in mouse, frog and human systems and is highly expressed in the basal cells of many human epithelial tissues. p63 deficient mice have defects in the apical ectodermal ridge essential

to limb development and the mice have truncated limbs. Over expression of p63 in normal human epidermal keratinocytes up-regulates markers specific for keratinocyte differentiation. This study investigated how radiation affects the expression of p63 protein in normal differentiating cultured human lens cells by western analysis. p53 protein levels do not change significantly with lens cell differentiation. However, a slight increase in p63 is seen at 12 days of growth as the cells begin to differentiate. After radiation exposure of epithelial and fiber cells, a dose-dependent increase was seen in p53. Further research to investigate the significance of this observation and to understand the role of p53/p63 in the human lens model will be pursued. Additional information will be gained if a phosphorylated p63 antibody is utilized to detect newly synthesized or activated p63 in response to radiation damage.

Mapping and Sequencing of Mammalian Genes for Comparative Analysis.

MAYA YANOVER (Santa Monica College, Santa Monica, CA 90405) **JAN-FANG CHENG** (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). Coding sequences in humans comprise less than 5% of the entire genome. Non-coding, cis regulatory sequences, located within the other 95% of the human genome, that do not code for proteins, determine the level, location and chronology of gene expression. There has been minimal identification and characterization of these regulatory sequences despite their importance, partially due to the difficulty in distinguishing regulatory sequences from other non-coding sequences. DNA regulatory sequences tend to be conserved through evolution and likely serve important functions, or disappear as organisms evolved. Ultimately, the information derived from sequencing other mammalian genes will allow researchers to generate cross-species (i.e. human/mouse) comparative analyses on human gene sequences acquired from the Human Genome Project. The comparative analyses provide new dimensions to our understanding of the evolutionary history of the human genome as has affected both genome organization and chromosomal structure. In contrast, studies of highly conserved non-coding sequences found in both species increases the understanding of important regulatory elements and roles for gene expression. The angiotensin I-converting enzyme (ACE) gene encodes for an enzyme involved in catalyzing the conversion of angiotensin I into a physiologically active peptide, angiotensin II. Angiotensin II, a potent vasopressor, controls blood pressure and fluid-electrolyte balance. The mapping and sequencing of the ACE gene in *Didelphis virginiana*, *Atelerix albiventris*, and *Oryctolagus cuniculus* allows for comparison with the human ACE gene sequence. High levels of sequence homology help to identify biologically active regions of a genome and distinguish important regulatory sequences from nonfunctional surrounding sequences.

Molecular Analysis of the Microbial Community Structure in Chromium Contaminated Sites Before and After *In Situ* Bioreduction Stimulation by Lactate Injection.

RAMÓN MARTINEZ (University of Puerto Rico, Mayaguez, PR 00681) **TERRY C. HAZEN** (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). Chromium is one of the most abundant elements on the Earth's crust. It is one of the most common contaminants because of its use in many industries. The major concern about waste containing chromium is the effects that it has on human health. Bioremediation may be the answer to reduce chromium to a less hazardous state by adding carbon source as electron donor. The main focus of this research is to analyze the microbial community structure using molecular approaches in chromium contaminated soil from Hanford, Washington, before lactate biostimulation. Soil enrichments, and small scale microcosms were used to obtain DNA from low biomass samples. 16S rDNA amplicons using Domain and specific group primers were obtained, and T-RFLP and DNA micro array technologies were used to analyze the microbial community. The molecular methods in this study demonstrated the low biomass content of the samples, the non-complex community structure, and the dominance of members of the Proteobacteria and gram-positive bacterial divisions. Geobacter and were two of the metal-reducers found in both the enrichments and small scale microcosms.

On the path to Structural and Functional Analysis of Nudix

CLAUDIA KLIEMANN (California State University Fresno, Fresno, Ca 93714) **STEPHEN R. HOLBROOK** (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). Prior to protein structural and functional analysis, proteins are crystallized following purification. The emphasis of this work falls into the purification and crystallization phase. The proteins of interest are from the bacterium *Deinococcus radiodurans*, the most radiation-resistant organism discovered. Collectively they are known as the Nudix proteins, 24 have been identified in the *D. radiodurans* genome. Though found in other organisms these specific ones are our focus because of their distinct ability to repair DNA in *D. radiodurans*. Purification involved

induction of *Escherichia coli* cells containing plasmid with Nudix genes. Initially the cells were incubated overnight to allow for induction, followed by sonication to lyse cells and access proteins. Centrifugation was used to settle out other cell components not involved in protein purification. Ion exchange column chromatography was next using a HiTrap 5ml SP HP column and a HiTrap 5ml Q HP column on the BioCAD Sprint, Perfusion Chromatography System. Once purification was achieved, the protein was combined with initial screen methods from Hampton Research, after which conditions were optimized for crystal formation. This work will hopefully lead to profiling the sequence basis and specific function and will also help in deciphering phylogenetic and evolutionary relationships among the Nudix proteins.

Positron Emission Tomography as a Diagnostic for Prostate Cancer. SUPIN CHEN (University of California Berkeley, Berkeley, CA 94720) WILLIAM MOSES (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Nonclinical cancer cells are present in the prostate of 40% of men over the age of 50; 4% of men over 50 have clinically significant prostate cancer. A low cost PET camera is being built to detect prostate cancer, stage the level of the disease, and guide its treatment. The camera will consist of two curved detector banks, each having two rows of detectors. The detector modules will be directed toward the center of the camera in order to increase resolution in the region of the prostate. Although average- to large- size patients will not be fully encircled by detector rings, causing incomplete sampling due to side gaps, simulations predict minimal blurring in the 10 cm diameter central region for a wide range of patient sizes. The prostate PET camera will use only a quarter of the number of detectors of a conventional PET system and have a significantly lower price. However, the camera will have nearly twice the solid angle coverage for a central point source compared to a conventional 2-D PET camera, because the detectors will be mounted onto elliptical arcs that are placed close to the patient. Thus, improved detection efficiency near the prostate is expected at lower cost.

Quantification of Phospholipid Fatty Acid Analysis. NAOMI NDAVU (Warren Wilson College, Asheville, NC 28815) SHARON BORGLIN (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Membrane lipids are extremely diverse and are used as markers for classification and identification of microorganisms. Predominant membrane lipids such as phospholipid fatty acids (PLFA) are useful in determining the types of microorganisms in a system (1), giving indications of the physiological status of the microbial community (2), and providing a means for estimating microbial biomass (3). This information is valuable in evaluating changes in community structure and status during remediation or treatment activities, and evaluating the microbial status of natural systems. The reliability of PLFA extraction and analysis depends on the experimental methods used to extract fatty acids. If large percentages of lipids are lost during extraction, interpretation of results will be affected. To understand recovery efficiencies, phospholipids were extracted from pure, freeze-dried samples of *Azotobacter vinelandii*, a bacterium (Azo), and *Spirulina plantensis*, an alga (Spir). The Azo and Spir samples showed a consistent pattern for all masses used. However, mass of fatty acids recovered per gram of sample did not increase linearly with larger masses. Both cell types have a complex relationship between mass and fatty acid response, possibly caused by saturation of extraction procedure when using high concentration samples, causing a loss of lipids. Further work is needed over a larger range of masses to completely characterize quantitative recovery. Further evaluation of the technique was accomplished by optimizing the methylation step using a standard phospholipid, palmitic acid. The result showed that decreased temperature and shorter incubation times improved recovery.

Structural Aspects of Transcriptional Activation. ELIZABETH LEVIEN (University of Florida, Gainesville, FL 33612) GERRY MCDERMOTT (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Although proteins are fundamental to our understanding of biology, ironically, few areas of study leave scientists with such an incomplete picture of their true nature than do proteins. Researchers are pursuing the enormous task of furnishing the complete account of the roughly 30,000 genes encoding all of life's proteins. DNA must first be transcribed into RNA polymers before being translated into the unique amino acid sequences of proteins. Transcription is highly regulated by an enzyme known as RNA Polymerase II (Pol II) and a system of proteins formed upstream of the DNA sequence to be transcribed known as the Pre-Initiation Complex (PIC), which is comprised of transcription factors, activators, and coactivators. Understanding transcription and its mechanisms of interactions relies on determining the native biological structure of protein and the specific way its amino acid sequence folds when conducting its specific cellular functions. cAMP (cyclic adenosine monophosphate) Responsive Element Binding Protein, CREB,

is a protein associated with transcription and stimulates target gene expression. Of particular interest to researchers is CREB's interaction with coactivators and the PIC. Although it is well known that an increase in cAMP production encourages the binding of CREB to its coactivator CBP (CREB Binding Protein) and amplifies subsequent gene expression, little is known about the structural basis of this interaction. Additionally, the proposed interaction between CREB and the transcription factor TFIIA is of great interest. One method commonly used in structural biology is the use of X-rays to yield a three dimensional structure by way of an X-ray diffraction pattern from a single protein crystal. Preliminary results have indicated an interaction exists between CREB and TFIIA, though no crystal structures have been produced as of this printing. Future work includes the possible coexpression of these two proteins in an attempt to aid purification and crystallization, as well as the continuing of current techniques.

The Role of XPG in Short-Patch BER: Stimulation of Polymerase Beta. RACHEL MCMULLEN (Knoxville College, Knoxville, TN 37921) BRETT M. HALTIWANGER (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

XPG (xeroderma pigmentosum gene) is a protein that has been studied in the Cooper lab since 1994. XPG was initially characterized by its enzymatic role in NER (nucleotide excision repair) but new studies have shown that there is a non-enzymatic role in BER (base excision repair). The role of XPG was examined in BER focusing on its role in stimulation of polymerase beta (pol b). Various assays were conducted to test for interactions of XPG with different proteins, including NTH1, APE1, and pol b. It is becoming clear that the role of XPG in BER is important. Analysis of these assays provided results that showed there was stimulation of Pol b and other proteins by XPG.

Three-Dimensional Histopathology of the Mammary Gland. ABBEY HARTLAND (Shasta College, Redding, CA 96049) CARLOSORTIZ DE SOLORZANO (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Breast cancer researchers today are faced with the extensive task of discovering and describing the mechanisms that drive the initiation and progression of mammary cancers. To correctly define these mechanisms, they must be studied in the context of the tissue where they appear and develop. Several techniques exist to detect or quantify proteins and genes involved in this neoplastic process, however, none have been able to both identify and effectively preserve these chemicals within their histological context. In response to these difficulties, our laboratory has developed a computer-assisted microscopy system to transform serial sections of tissue into a three-dimensional (3D) image, thus allowing us freedom to both identify breast cancer markers and to visualize the context where these markers are found in vivo. This system was utilized to reconstruct the mammary ductal tree of a 6-week-old wild-type female mouse. Using current immunohistochemical techniques, we mapped three major proteins known to have a crucial role in the normal development of the gland: estrogen receptor (ER)- α , progesterone receptor (PR), and the growth factor receptor neu. This 3D map can then be compared against reconstructed mammary tissue of a transgenic strain of mice known to develop mammary tumors, thus enabling us to determine changes in the morphology and the pattern of receptor expression associated with cancer initiation and development.

Transformation of *C. elegans* with Chromosome-binding Green Fluorescent Protein Fusion Protein Using Microparticle Bombardment. A RAM KIM (Santa Monica College, Santa Monica, CA 90405) PETE CARLTON (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

In order to explain the mechanisms chromosome pairing, it is helpful to understand the dynamics of meiotic chromosomes. pPC01, the plasmid holds F41H10.10 and GFP fusion, was constructed for live imaging. By transformation of *C. elegans* (worm) with the plasmid, we will be able to visualize chromosomes in vivo as they are undergoing the process of meiosis. However, injecting the DNA plasmid will cause repetitive arrays and result in silencing in a germline. Microparticle bombardment has been shown to produce low copy integration of transgenes. these transgenes are not silenced, so the result is stable germline transformation. We bombarded unc-119 mutant worms with gold particle carrying pPC01 to get transformation. We got some rescued unc-119 worms, but as we expected they did not have expression for pgl-1 GFP : : F41H10.10 fusion. We did not get transformants by ballistic bombardment. We will keep working on this project and in the future, we might get transformation.

A Putative Pyruvate: Ferredoxin Oxidoreductase Gene in *Chlamydomonas reinhardtii* is Expressed During Fermentative Hydrogen Production. JONATHAN MEUSER (University of California at Davis,

Davis, CA 95616) MARIA GHIRARDI (National Renewable Energy Laboratory, Golden, CO 89401).

The unicellular green algae *Chlamydomonas reinhardtii* has received considerable attention both as a model for photosynthesis and as a potential renewable source of hydrogen fuel. As we learn more about the biological pathways that produce hydrogen in *C. reinhardtii*, hydrogen production may be improved or produced from more varied substrates. *C. reinhardtii* can produce hydrogen anaerobically in the light and dark. Hydrogen photoproduction pathways are well studied, whereas little is known about dark anaerobic hydrogen producing pathways. Furthermore, while *HydA1* is likely involved in photoproduction, the function of *HydA2* in algal hydrogen production is unknown. The goal of this work was to identify the link between fermentative carbon metabolism in *C. reinhardtii* and dark, anaerobic hydrogen production. One product of fermentative carbon metabolism is pyruvate. In several species of anaerobic microbes, the decarboxylation of pyruvate to acetyl-coA by pyruvate:ferredoxin oxidoreductase (PFOR) is linked to hydrogen production. The completion of the *C. reinhardtii* genome has allowed us to utilize a bioinformatics approach to identify a putative PFOR ortholog. A search of the *C. reinhardtii* genome identified a single putative protein with four orthologous functional subunits that showed high protein similarity to other known PFOR enzymes. An improved gene sequence was completed. Finally, Northern blot data of RNA from anaerobically induced cells showed that the predicted PFOR gene is expressed. Moreover, expression revealed that the putative PFOR is transcribed concomitantly with *HydA1* and *HydA2*. The identification of the *C. reinhardtii* putative PFOR gene and evidence of its coexpression with *HydA1* and *HydA2* suggests fermentative carbon metabolism and dark, anaerobic hydrogen production may be linked via ferredoxin. With further work the PFOR activity and relation to hydrogen production may be definitively shown, potentially enabling improvements in the yield of biological hydrogen production from *C. reinhardtii*.

Electronic Characterization of Carbon Nanotubes. MONICA SAMEC (University of Toronto, Toronto, ON M4T 1S6) RANDY ELLINGSON (National Renewable Energy Laboratory, Golden, CO 89401).

Single-walled carbon nanotubes (SWNTs) show great promise for a variety of applications. However, the field is still young and has major challenges. One challenge is that particular types of SWNTs cannot be individually synthesized or purified in an appreciable quantity. As different types of tubes have vastly different electronic structures, attributing a signal to one particular tube type can be difficult. The fact that they are usually bundled with many other types of SWNTs further complicates their electronic properties. In this project, photoluminescence spectroscopy was used to assign SWNT types to the emission and absorption peaks, observe the effect the presence of these SWNTs have on photoluminescence of sodium dodecyl sulfate (SDS), and to analyze the effectiveness of the separation of high-pressure CO conversion (HiPco) SWNTs suspended in 1% SDS in deuterated water (D₂O). It was found that use of a swing bucket rotor rather than an angle rotor in the centrifuge leads to more effective SWNT solubilization in SDS. Many of the emission and some absorption peaks could be assigned to specific tube types. Preliminary evidence suggests that carbon nanotubes may enhance the photoluminescence of SDS. Further work will focus on validating of these recent findings.

Automating the Purification of Protein Complexes using Magnetic Beads for High-Throughput Functional Proteomics. MARSHALL MILLER (Appalachian State University, Boone, NC 28608) PETER HOYT (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The functional products of genes are the proteins and the next step towards understanding cellular physiology lies in understanding the interactions of its protein complexes. To accomplish this goal, laboratory procedures for isolating and purifying protein complexes must be adapted in order to account for the elevated throughput needed to analyze the vast number of protein complexes present. We have adapted a magnetic-bead based affinity system to a liquid handling robot, to perform automated and rapid purification of proteins from bacteria. The process begins with samples that are bead milled to lyse cells. Bead milling utilizes zirconium/silica beads, agitated at a high speed, in a lysis buffer. This is a particularly adept process as it is a closed lysis system (nothing is added or removed from the samples and thus there is no chance for cross-contamination between samples), it applies equally well to most cells and tissues, and it is also an automation-compatible process. A protocol for protein isolation and purification was adapted to an 8-tip MultiPROBE IIHT EX TM liquid handling robot run by WinPrepTM. This adaptation allows for 96 different samples to be processed simultaneously and allows for isolation and purification of their associated proteins in complexes. Proteins are expressed with one or more fused affinity-tags consisting of six consecutive histidine resi-

dues (6-His). Our test system utilizes Ni-NTA Magnetic Agarose Beads to bind 6xHis-tagged protein complexes in *Escherichia coli* (*E. coli*). After ensuring that the beads are free of foreign proteins by washing the beads with a lysis buffer, the beads are robotically added to a bacterial lysate and allowed to bind. The beads can then be 'pulled down' to a magnetic support tile on the robot. The bead-bound proteins can then be washed with a lysis buffer remove impurities. Finally the purified protein complexes are eluted with a buffer containing high-concentration imidazole. GFP visualization showed the process was uniform across samples and that the volume of protein in the elutant is sufficient for downstream analysis. An SDS-Polyacrylamide Gel Electrophoresis assay (used to access purity) indicated that samples were at least 95% pure. The end product of this process, the eluted proteins, will later be utilized for protein identification by Mass Spectroscopy.

Elemental Characterization of Skeletal Remains Using Laser-Induced Breakdown Spectroscopy (LIBS). KIM COLLINS (Maryville College, Maryville, TN 37804) ARPAD VASS (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

When presented with skeletal remains from a possible crime scene, the forensic anthropologist and/or medical examiner must identify the remains as human or animal. A positive identification as human initiates legal investigation whereas classifying the remains as animal does not. In forensic consultations, approximately 25-30% of forensic cases are nonhuman. Currently, the methods for this type of identification rely heavily on the availability of a mammalian osteology specialist. Separation of nondiagnostic or extremely fragmented remains can prove nearly impossible to classify even to experienced osteologists. Macroscopic and microscopic evaluations are the traditional methods used for identification. Both methods have a margin of error dependent on the experience of the specialist. In addition, microscopic evaluations are destructive to the specimen and time consuming. Given the legal ramifications involved in accurate identification of skeletal remains, a more reliable means by which to distinguish human from animal remains is desirable. This research utilized Laser-induced breakdown spectroscopy (LIBS) for the characterization, and subsequent separation, of elemental bone composition profiles from several commonly recovered mammalian species. LIBS is an established, versatile method of determining elemental compositions. Laser pulses delivered to the sample form plasma containing the emission spectra of the atomized elements. Plasma light collection, followed by spectroscopic detection, permits element identification through their unique spectral signature. A femur or tibia of a rabbit, pig, sheep, bear, cow and white male was selected from the William M. Bass Forensic Skeletal Collection at the University of Tennessee and analyzed with LIBS. The cortical shaft was shot with a Nd-Yag laser in a representative region for adequate sampling. Each sample was shot 100 times at a power of 40 mJ creating a spectrum of elemental peaks from wavelength 200-800 nm. Initial comparisons of spectral data showed elemental differences between human and animal bone. Pending further analysis, identification of elemental differences using LIBS may provide a more efficient method of bone classification.

Genomic Characterization of Below Ground Ecosystems to Climate Change. JAMIE WIEGEL (University of Virginia, Charlottesville, VA 22904) LEE GUNTER (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Below ground processes are significant when predicting ecosystem responses to global change. Genomics approaches promise to help revolutionize the study of belowground communities by giving researchers insight into the mechanistic understanding of climatic change at the genetic level. These approaches are being applied in the newly established OCCAM facility at Oak Ridge National Environmental Research Park, a unique facility that examines the interacting effects of temperature, precipitation, and [CO₂] on the composition and productivity of an old-field plant community. In order to quantify the belowground competitive interactions among genes, consistent quantitative methods of DNA extraction, as well as a consistent method of Real-Time PCR analysis of amplified gene targets from each of 7 target plant species used in the study is being developed. Previous analysis of quantification data established that the Quiagen DNeasy protocol provides consistently clean DNA template with reasonable yields (2µg to 10µg starting material) among pure species. To further refine the protocol for potentially low biomass yields mixed environmental samples, variable amounts of starting material (5mg to 20mg) were used to extract DNA from freeze-dried tissue. It was predicted that a linear correlation between increasing amounts of starting material and DNA yield would be seen. The data, however, showed variable results within species and, thus, remain inconclusive. Polymerase Chain Reaction (PCR) was used as a species-specific molecular assay with primers designed to specifically amplify genes in the 7 target species: *Andropogon virginicus*, *Dactylis*

glomerata, *Festuca pratensis*, *Lespedeza cuneata*, *Plantago lanceolata*, *Solidago canadensis*, and *Trifolium pratense*. Reaction conditions were optimized by varying salt, primer, and template concentrations in the reaction mix, with 1.5mM Mg²⁺ and 0.67μM primers providing the optimal reaction conditions for most species. Primer specificity was tested by using both target and non-target species templates in combination with the 7 target species specific primers. In all cases, species-specific primers amplified only the target species and mixed templates containing the target species but did not amplify the non-targets. PCR analysis with additional species mixtures and refinement of DNA extraction protocols will continue, and the results will be used to develop Real-Time PCR assays for each target species.

Integrating a Network Monitoring System into a Computing Infrastructure. AMELIA JAMISON (*Southwest Tennessee Community College, Memphis, TN 38134-7693*) MICHAEL GALLOWAY (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The Life Sciences Division's Genome and Systems Modeling Group maintains a complex environment of computing and network resources to accomplish its objectives. Section staff, other ORNL staff and users worldwide depend on these resources being available and on high performance. For these reasons, the integration of a system and network monitoring system into the computing infrastructure in LSD/GASM is necessary. A system monitor would check the states of the computing and network resources, provide notifications to responsible staff members, and enormously benefit in providing even higher levels of reliability, performance and system uptime. To achieve this objective, research evaluating several software packages was made. In an effort to compare network monitors for features, the World Wide Web provided live and sometimes interactive demonstrations of products available. Available open source software was evaluated (<http://www.opensource.org/dos/definition.php>) in order to determine which, if any, would meet the needs of the department. Open source software allows users to implement them with little or no cost and gives access to the source code that can then be modified as needed to meet the specific needs of the user. The software packages were installed, configured for the GASM computing environment, and then evaluated in their effectiveness for providing accurate, timely and understandable results. As a result of reviewing several possible applications, Nagios (<http://www.Nagios.org>) and Cacti (<http://www.raxnet.net/products/cacti/>) together provided a complimentary view of the GASM computing environment. While Nagios provided a very robust tool for monitoring system and network services, host resources, etc., and has a sound tool for managing contact notifications, Cacti provided a very graphical view into system and network performance, maintaining a long term database of relevant parameters. Nagios and Cacti, working together, facilitate the job of the network administrator. Before implementing the system monitor the responsible staff would have to individually log on to each computer to check out each service or application. These monitors eliminate a lot of time that would need to be spent checking each host. They also provide accurate information and decrease the likelihood of error.

MALDI-TOF Mass Spectrometry Detection of Mutations in the Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) Gene. CAROLINE MARTZ (*Knox College, Galesburg, IL 61401*) CHUNG HSUAN CHEN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*). Cystic fibrosis, an autosomal recessive disorder caused by mutations in the cystic fibrosis transmembrane conductance regulator (CFTR) gene, affects more than 25,000 Americans. Over one thousand mutations causing the disease have been identified; screening for these mutations, however, is difficult and time-consuming using conventional techniques. The goal of this project is to develop a high-throughput screening system for detecting multiple mutations in CFTR using matrix-assisted laser desorption and ionization time-of-flight (MALDI-TOF) mass spectrometry. Locus-specific PCR was utilized to amplify regions 508 and 1282, commonly mutated in cystic fibrosis. The CFTR amplicons were denatured, attached to a nylon membrane, and hybridized with mass-tagged, biotinylated probes. The mass tags of the probes for the normal and abnormal sequences at a particular locus differed by five base pairs. Hybridization of the probe to the amplicon was confirmed using a colorigenic biotin-streptavidin-alkaline peroxidase reporter system, allowing optimization of hybridization conditions. Hybridization to a normal versus a mutated sequence in the amplicon was distinguished via effective mass using MALDI-TOF mass spectrometry. Preliminary results demonstrate stringency and specificity of hybridization on nylon membranes via colorigenic detection. Future work will include optimizing hybridization conditions for amplicons attached to derivatized glass slides, a substrate more amenable than membrane to detection with MALDI-TOF mass spectrometry.

RT-PCR and Preliminary Heteroduplex Analyses of ENU-induced Prenatal-Lethal Mutations in the Mouse *Herc2* Gene. DOMINIQUE FONTANILLA (*Carleton College, Northfield, MN 55057*) MITCHELL KLEBIG (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

N-ethyl-N-nitrosourea (ENU) is a potent non-specific point mutagen that can produce both recessive and dominant forms of loss-of-function (null), hypomorphic, and gain-of-function mutations. In previous studies, seven recessive ENU-induced mutations in mice were found to exhibit a juvenile development and fertility (*jdF2*) phenotype, which is characterized by stunted growth, jerky movements, female semisterility, male sterility, and shortened life spans. Deletions of the *Herc2* gene (i.e., null mutation) also result in the *jdF2* phenotype. Three of these mutations were shown to be alterations in the mouse *Herc2* gene, which produces a protein potentially involved in vesicular protein trafficking and degradation pathways. Interestingly, four additional recessive ENU-induced mutations at the *jdF2/Herc2* locus cause prenatal lethality, which is more severe than the null phenotype. The objective of this study, therefore, is to genetically characterize *Herc2374SJ*, *Herc21193SJ*, *Herc21881SJ*, and *Herc2982SJ*, the four ENU-induced alleles that cause prenatal lethality. As indicated by the reverse transcription-polymerase chain reaction (RT-PCR) experiments in this scientific investigation, no size alterations (indicative of, e.g., exon loss) were found in the *Herc2* gene. Initial heteroduplex analyses on these RT-PCR reactions look promising for potential single-base pair mutations in significant regions of *Herc2*. Determining specific gene mutations in these *Herc2* ENU-induced alleles will be fundamental for elucidating the role of *Herc2* in biological systems and potentially identifying functional domains/motifs of the protein essential in prenatal development.

Testing of a Novel Antiviral Drug Candidate. JOSHUA MOUNT (*Roane State Community College, Harriman, TN 37748*) TANYA KURITZ (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The human body responds to viral infections by launching cascades of immunological reactions aimed at elimination of the virus. The interferon system is a part of innate immunity and is the body's natural antiviral defense. Innate immunity is the first barrier to infection and is conferred through the action of interferons alpha and beta (IFN α/β), and interleukins (IL) produced by natural killer cells and macrophages; the body's defense against viral infection is also dependent on the induction of an adaptive immune response [1]. Compound M is a novel antiviral drug candidate which is able to induce interferon [2]. Compound M was also reported to upregulate biosynthesis of cytokine transcription in human cell cultures, to increase levels of interferon and cytokines in murine blood serum, and to induce Ca²⁺ transients in human cell culture [2]. This project was aimed at the characterization of Compound M's ability to induce innate immunity in three human cell lines, erythroleukemia (K-562), monocyte (THP-1), and human foreskin fibroblasts (HFF). The effect of Compound M was assessed in vitro by (1) calcium signal imaging using fura-2 and fluo-3 Ca²⁺ binding dyes, and (2) reverse transcription-polymerase chain reaction using sets of cytokine-specific primers. It was found that THP-1 and K-562 cells may not be used in Ca²⁺ signaling studies because they fail to adhere to the poly-D-lysine treated support. HFF cells did not exhibit a response to nicotine (a control stimulus) probably due to the lack of necessary receptors. In the RT-PCR experiments, we found that IL-1 α was synthesized four to six hours after exposure of THP-1 cells to Compound M.

The Detection of Biological Agents Through the Use of Polymerase Chain Reaction (PCR) and Application to Biochip Detection. STEPHEN ANDERSON (*ETSU, Johnson City, TN 376303*) GUY GRIFFIN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Polymerase Chain Reaction (PCR) is the most widely used method of DNA amplification. PCR is the repetitive bi-directional DNA synthesis via primer extension of a region of nucleic acid. PCR amplification of a template requires two oligonucleotide primers, the four deoxynucleotide triphosphates (dNTPs), magnesium ions and a thermostable DNA polymerase. This research involved the adaptation of PCR to a field setting in the detection of biological warfare agents. Lambda phage DNA genome is being used as a model system. Success of PCR amplification is assessed through agarose gel electrophoreses using ethidium bromide to stain the product and ultraviolet light detection. Once established that the unmodified primers for Lambda work in the PCR amplification, then attempts to amplify using modified primers, i.e. Cy-5 and Biotin labeled primers are being undertaken. Modifications to reaction conditions are occasionally necessary to obtain amplification of these primers. Detection of Cy-5 labeled amplicons was accomplished using a He-Ne laser after agarose gel electrophoresis. The Biotin labeled amplicons are captured in streptavidin coated micro wells and detected using Cy-5-labeled oligonucleotide probes. The results of this research

will feed directly into the field hardware, containing the miniature PCR device and Biochip, which is currently under construction.

A Comparison of Two Gamma Ray Spectroscopy Systems for Quantifying Radioactive Material in the Body. JAMES RIVARD (*Central Washington University, Ellensburg, WA 98926*) TIM LYNCH (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Two portable gamma ray spectroscopy systems were evaluated during the course of this study: one using a high purity germanium (HPGe) detector and another using a sodium iodide (NaI) detector. The efficiency, resolution, background levels with and without shielding material, minimum detectable activities (MDA), decision levels, as well as advantages and disadvantages of the two detection systems were compared. Measurements were performed inside and outside of shielded rooms on both bottle-manikin-absorption (BOMAB) phantoms and human subjects. Data for HPGe and NaI detectors was analyzed separately. MDA and decision level results were calculated for ^{133}Ba , ^{60}Co , ^{137}Cs , ^{152}Eu , and ^{40}K based on ten-minute counts. The average MDA and decision levels results for the HPGe detector were a factor of five smaller than the NaI detector results for all of the nuclides inside and outside of shielded rooms. The estimates of radioactive material in BOMAB phantoms were correctly estimated within 10% inside shielded rooms and within 30% in unshielded environments. However ^{40}K could not be properly estimated with a ten-minute count time. The average MDA and decision level values calculated for all the nuclides with both the HPGe and the NaI detectors were well below the annual limits on intake. The HPGe detector can resolve multiple energies better than NaI detector; however the NaI detector has better efficiency, which reduces the count time necessary to achieve adequate results. However, the HPGe detector requires liquid nitrogen. The NaI detector was found to be adequate for emergency applications during this preliminary study, given that resolution and rapid temperature changes are not an issue. Future work may include a study to investigate how well estimates of lung and organ activity can be made with a single detector.

A Study on the Use of Living Systems, or Biosentinels, for Monitoring and Detecting Toxins and Pollutants in a Marine Environment.

SARA WYNVEEN (*Lane Community College, Eugene, OR 97401*) KAREN STEINMAUS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The ability to detect and monitor the presence of toxins and pollutants in marine environments has become increasingly important in both environmental and national security applications. Researchers at the Pacific Northwest National Laboratory are investigating the use of living systems - primarily bivalves (mussels, clams, oysters) - as possible indicators of contaminants in marine environments. Because bivalves are filter feeders, their accumulation and prolonged retention of materials makes them optimal organisms for sampling. Under an ongoing research effort, Marine Sciences Laboratory staff scientists are involved in an investigation into the use of bivalves native to coastal Pacific Northwest waters to detect and monitor the presence of toxins and pollutants at levels lower than are easily detected by instruments. A critical transition area in the coastal zone exists in which organic chemicals, metals, and bacteria are transported through estuaries from fresh to saltwater. Little is known about the geochemical behavior of these materials as they travel between freshwater and saltwater systems. The present study was established to examine an estuarine environment, represented by a freshwater tank providing partial flow into a saltwater tank established in the laboratory, modeling the transition from fresh to salt water in a coastal zone. Low doses of chemicals were introduced to the freshwater tank, and were thereby delivered to the saltwater tank in even lower concentrations. Water and tissue samples from both the salt and freshwater bivalves were collected prior to the introduction of chemicals, throughout the exposure time, and after dosing had ceased. These samples were subsequently analyzed for indicators of the contamination. A separate experiment is currently in process to evaluate behavioral indicators in the presence of toxins/pollutants. A separate saltwater tank has been set up and local organisms have been collected and placed into the test system. After a baseline period of adjustment and observation of behavior among the organisms, small amounts of chemicals were introduced and behavioral changes monitored and recorded to find observable behavioral indicators of the contaminant.

Acetylcholinesterase Activity in Tissues from Rats Exposed to Mixtures of the Organophosphorus Insecticides Chlorpyrifos and Diazinon. MELISSA HINMAN (*Whitworth College, Spokane, WA 99251*) CHARLES TIMCHALK (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Chlorpyrifos (CPF) (O,O-diethyl-O-[3,5,6-trichloro-2-pyridyl]-phosphorothioate) and diazinon (DZN) (O,O-diethyl-O-[2-isopropyl-4-methyl-6-pyrimidinyl]-phosphorothioate) are two of the most commonly used

organophosphorus (OP) insecticides. When metabolized, CPF and DZN have the ability to target and inhibit the enzyme acetylcholinesterase (AChE), which makes them effective insecticides, but also causes them to be toxic to non-target species, including humans. There is great potential for human exposure to mixtures of these two insecticides as they are often used together in agricultural settings, but little is known of how interactions between the two insecticides might affect AChE activity. The purpose of this study was to characterize the resultant AChE activity following Sprague-Dawley rat exposure to a single dose of each chemical separately or in a mixture. Rats were exposed to DZN and CPF at doses of 15, 30, and 60 mg/kg body weight and were sacrificed at 0, 3, 6, 12, and 24 hours post-dosing. The plasma, red blood cells and brain were collected and a modified Ellman method was used to measure AChE activity in the tissues. It was found that the enzyme was inhibited most in plasma, followed by red blood cells and then the brain. In general, the level of enzyme inhibition followed this pattern: CPF+DZN>CPF>DZN. Preliminary analysis of the data seemed to show that the interaction between CPF and DZN was more complex than simple additivity.

An Environmentally Friendly Preparation of Deoxyribonucleotides and Ribonucleotides for Use in Structural Heteronuclear NMR Studies. KIFFANY PEGGS (*University of Tennessee at Knoxville, Knoxville, TN 37916*) NANCY ISERN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The production of isotopic-labeled deoxyribonucleotides is an essential step in the preparation of short oligomeric sequences for DNA repair studies. Isotopic labeling increases the number and type of NMR experiments that can be performed in DNA structure calculations. Presently, the simplest method for production of isotopically labeled deoxyribonucleotides is through the isolation of labeled cellular nucleic acids. The current procedures for DNA and RNA isolation include the use of chemicals such as phenol, isoamyl alcohol, and chloroform. These chemicals can be harmful to the environment and harmful to the researcher. Furthermore, disposal of spent reagents can be expensive. This paper illustrates an alternate method developed for simultaneous DNA and RNA isolation from bacterial cell cultures. This method takes advantage of: 1) the negative charge on nucleic acids; 2) the ability of a chelating agent to remove positively charged contaminants from solution; 3) the ability of heat and detergents to denature and solubilize contaminating protein; and 4) the ability to precipitate nucleic acids from solution using ethanol and salt. The isolated cellular nucleic acids can then be hydrolyzed and the individual ribonucleotides and deoxyribonucleotides purified using chromatography. This procedure is comparable in efficiency to the phenol chloroform extraction procedure currently used to date by researchers.

Bioencapsulation of Halogenated Acetic Acids in Artemia and Short-Term Feeding Trials to Japanese Medaka (*Oryzias latipes*). STACEY REED (*University of Tampa, Tampa, FL 33606*) IRV SCHULTZ (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Halogenated Acetic Acids (HAA'S) are one of the important classes of by-products that come from the disinfection of drinking water. Dichloroacetic acid (DCA) and dibromoacetate (DBA) are among the dominant forms. Past fish studies have used water exposure as the treatment route, yet an oral exposure would be more applicable to human health effects as humans consume drinking water. Since DCA and DBA are highly water-soluble, microencapsulation and bioencapsulation was explored in order to prevent leaching of the chemicals before the fish consumed them. Five treatment groups were used (high and low dose of both DBA and DCA, as well as a control) in order to see if bioencapsulation would show levels of DCA and DBA in fish tissue. Experiments demonstrated that most of the Artemia would uptake similar amounts of DCA and DBA. Cold temperatures were explored as a method of storage and found unacceptable. Artemia uptake fluctuated daily, yet should not be a major concern in a long-termed study. Bioencapsulation was demonstrated to be an effective method in orally dosing Japanese medaka.

CEC Method Comparisons. KATHERINE STRACHAN (*University of Iowa, Iowa City, IA 52242*) GLENDON GEE (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Cation-exchange capacity (CEC) is an important chemical property of soil, required as an input parameter in reactive-transport models, used to predict contaminant migration from buried-waste sites. Determining the CEC of a soil can be obtained using well-established laboratory procedures. Unfortunately, CEC values have been found to be method dependent and specifically affected by high residual salt concentrations, among other factors. A new method from Zachara et al. (2002) for determining CEC was evaluated at Hanford against two other methods, the Plemio and Rhoades procedure (1957) and EPA Method 9081 (1986).

This new method bathes each sample in sodium acetate, then sodium bicarbonate, and then deionized water until the electrical conductivity of the solution is less than five microseimens per centimeter. Fifty milliliters of deionized water is added to each sample and rotated for four hours. After centrifuging and extracting a water sample, ammonium chloride is added. The solution is rotated for another two hours and another liquid sample is obtained. The liquid samples are analyzed using Inductively Coupled Plasma Spectroscopy (ICP) analysis. When contrasting the three results, the measured CEC using EPA Method 9081 was consistently higher than the other two methods. The new method shows similar trends to the EPA Method 9081, but with consistently lower results. In summary, the Zachara et al. method and the EPA Method 9081 show similar trends, suggesting that CECs taken with the new method are relevant and may be less biased by salt loading effects than the other two methods. The results taken with the Plemio and Rhoades procedure are scattered and show little trends, suggesting that this method may not be as reliable for Hanford Site soils as the new Zachara method.

Characterization of Medium and Large Mammal Populations Within the Hanford Reach Riparian Habitat. KYRA EMORY (Columbia Basin College, Pasco, WA 99301) AMANDA STEGEN (Pacific Northwest National Laboratory, Richland, WA 99352).

The riparian ecosystem associated with the Columbia River provides habitat for a large variety of organisms, including mammals. Biological characterization of the riparian zone at the Hanford Site has been identified as one of the datasets that may be needed for the Tri-Party Agreement Records of Decision. These datasets provide evidence for cleanup decisions that will be made to be protective of the environment (DOE Order 450.1). In addition, biological characterization is part of the ecological risk assessment process for evaluating the likelihood of adverse ecological effects. This study was undertaken to characterize the medium and large mammal populations associated with the Hanford Reach riparian area. Thirty-four surveys were conducted at randomly selected points along the Columbia River shoreline from Vernita Bridge to the 100 B-C Area. These points were indicative of four types of riparian vegetation communities (Wormwood/Perennial Grass, Juniper, Willow, and Low Shrub-Cobble Association). Direct mammal sightings as well as indirect indicators such as scat, tracks, bed sites and foraging digs were utilized in these surveys to determine the species and location of mammals present in specific vegetation communities throughout the riparian zone. Deer, coyote, elk, porcupine and skunk signs were recorded within the communities surveyed. Deer and associated ungulate signs were most frequently observed (occurring in every community type) while skunk signs were observed the least (occurring in only one community). Porcupine and coyote sign were each found in two of the communities. It was concluded from the analysis of the gathered data that Juniper communities seem to be the most suitable riparian habitat surveyed, supporting both the highest density of sign and the greatest diversity of mammal types. The Low Shrub-Cobble Association was found to have a relatively high mammal diversity but the lowest sign density observed, suggesting that this community contains resources necessary to mammals but in quantities that are not great enough to support large populations. Conclusions could not be drawn from the Willow or Wormwood/Perennial Grass communities due to the small sample size obtained. Additional work will be necessary to further characterize mammal populations as well as other biota throughout riparian areas.

Characterization of the Human Mammary Epithelial Cell Membrane Subproteome. REBECCA GAALSZYK (Bethel College, St. Paul, MN 55112) DAVID CAMP, II (Pacific Northwest National Laboratory, Richland, WA 99352).

Cellular membranes are the boundary between intracellular components and their extracellular environment. This lipid bi-layer houses membrane proteins, amphipathic in nature, important for cell-cell interactions, mediation in the transport of ions and molecules, and for cell adhesion. The hydrophobic and hydrophilic nature of the proteins that allows them to be embedded in the membrane is the characteristic that makes them difficult to study. Characterization of the membrane subproteome of human mammary epithelial cells (HMEC) provides baseline identification for comparison of normal cells with cancerous or malignant cells. Identification of novel proteins creates potential biomarkers for early detection of cancer, allows for improved, targeted breast cancer treatments, and possible protein therapies. We report on the characterization of the membrane subproteome through basic membrane preparation using tryptic digestion, methionine enrichment, and biotinylation with PEO-iodoacetyl-Biotin. Fourier Transform-Ion Cyclotron Resonance (FT-ICR) mass spectrometry results show 995 accurate mass and time (AMT) tags for the membrane preparation, 472 AMT tags for the methionine enrichment, and 2,730 AMT tags for the

biotinylation. There is only minor overlap of the unique, identified AMT tags between all three methods. Although there is excellent coverage of the subproteome using the combination of the three methods, results demonstrate the need for further method development. Specific parameters such as denaturing conditions and chaotropic agents must be optimized for work with HMEC cells to increase membrane phospholipid and membrane protein solubilization.

Comparison of Sage Sparrow (*Amphispiza belli*) Territory and Non-territory Vegetation on the Hanford Site. LOVETTA MUL-LINS (MSU-College of Technology, Great Falls, MT 59405) MICHAEL SACKSCHEWSKY (Pacific Northwest National Laboratory, Richland, WA 99352).

The Hanford Site contains large blocks of late-successional shrub steppe, home to the sage sparrow (*Amphispiza belli*). Modification or removal of this habitat threatens the natural life cycle of the sage sparrow. Development of a Habitat Suitability Index (HSI) model will improve our ability to quantify the value of different potential habitat areas and will thus allow us to mitigate the impacts of environmental disturbance on this species. Research investigating the difference in vegetation between sage sparrow occupied and unoccupied territories will be used in the development of the HSI. Information obtained through the use of a Geographical Information System (GIS) was used to identify potential habitat areas. Field surveys within those potential habitat areas identified those that were or were not nesting territories. Vegetation characteristics were then compared in randomly selected plots within occupied and unoccupied territories. Percent canopy cover was measured in the following categories: annual grasses, both small and large perennial bunchgrasses, both annual and perennial forbs, shrubs, litter, and bare ground. Shrub species were identified and measured. The results indicated that areas selected for nesting by sage sparrows had greater amounts of sagebrush cover, native perennial cover, and less cover of non-native annual species than potential habitat areas that were not selected for nesting.

Dermal Absorption of Common Solvent Vapors in F344 Rats. CARON DORMAN (Washington State University, Pullman, WA 99163) KARLA D. THRALL (Pacific Northwest National Laboratory, Richland, WA 99352).

Benzene, toluene and xylene are all highly volatile compounds commonly found in paints, paint thinners, fingernail polish, lacquers, adhesives and gasoline. Due to their widespread occurrence in both occupational and nonoccupational settings, the possibility of their absorption into the body is high. While they are typically absorbed in the form of inhalation, they can also enter through the skin upon prolonged exposure. To determine the occurrence of dermal absorption by the body F344 male rats were used to simulate human exposure to the compounds and assessed using real-time breath analysis. The animals were dosed with 0.5- μ l of the neat compound into a 2.5-cm diameter aqueous exposure patch that had been adhered to their shaven backs. Once the animals had been dosed with the neat compound, their exhaled breath was taken through the real-time gas analyzer and assessed for the compound's concentration as the animal absorbed the compound through its skin over time. Upon the conclusion of a two hour exposure, animals were sacrificed using carbon dioxide gas and once again placed within the chamber to demonstrate the low levels of compound in the absence of their exhaled breath. This study is part of a larger effort being conducted to determine the health risks of compounds found in commonly used solvents.

Designing an *In situ* Chamber. MICHELLE PENN (Loyola University Chicago, Chicago, IL 60611) AMORET BUNN (Pacific Northwest National Laboratory, Richland, WA 99352).

Chironomus tentans (chironomids) are aquatic insects that are used during their larvae stages as water quality indicators. Groundwater plumes are entering the Columbia River above drinking water standards at the U.S. Department of Energy's Hanford Site in south central Washington. One particular area of concern is a strontium-90 plume located along the shores of the decommissioned 100 N reactor. In order to understand how these contaminants affect the aquatic organisms in the river, *in situ* chambers for chironomid larvae was developed to be deployed in large bore wells in the vicinity of 100 N reactor. In preliminary experiments, chironomid larvae were found to be substrate dependent organisms that have a better survival rate if the substrate is plentiful. Substrate provided surfaces for microorganisms to colonize, and the chironomids survived for over 7 days by feeding on the microorganisms living in the substrate. Results indicated that 25 chironomids per chamber would be an appropriate number of larvae for one chamber. The *in situ* chambers were designed to fit into a 0.3 m diameter groundwater well using a 10 cm diameter, 14 cm tall chamber made of 200 μ m plankton netting that would allow 25, 10 day old chironomids to live together

for over 7 days without harming each other or escaping. The chironomids and substrate in the chamber also had to remain completely submerged in groundwater and allow constant flow through the system. The two chambers were assessed using a 38 liter aquarium containing groundwater to act as the groundwater well. It was found that the design and construction of both in situ chambers fit into groundwater wells with a diameter of 0.3 m. The 3.0 mm mesh chamber appeared to be better suited for containing larvae and allowing groundwater and possible contaminants to flow through easily while remaining submerged. The 3.0 mm mesh chamber performed slightly better because it was sturdier than the 1.5 mm mesh chamber, which helped to keep chamber contents from seeping out between the lid and sides of the chamber. Overall, both chambers performed well because they were lined with the 200 micron mesh plankton netting, made of construction material that allowed the chambers to remain submerged, and contained enough substrate and food for the chironomids.

Developing a Habitat Suitability Index for the Hanford Site Sage Sparrow. NATHAN DIEHL (Florida State University, Tallahassee, FL 32306) COREY A. DUBERSTEIN (Pacific Northwest National Laboratory, Richland, WA 99352).

The sage sparrow (*Amphispiza belli*) is a Washington State listed or candidate species of concern. This obligate, shrub-steppe inhabitant, primarily dwelling in big sagebrush (*Artemisia tridentata*), is affected by the removal of sagebrush. In order to mitigate valuable habitat lost due to Hanford site activities, the development of a Habitat Suitability Index Model (HSI) is needed using the sage sparrow as the representative species to assess the relationship between territory and required resources. To develop an HSI, the territories of the singing males are mapped and the vegetative overstory and understory are measured. 500m transects are randomly generated throughout the Hanford site and singing males are identified along these transects and their territories mapped. Those areas where sage sparrows were not found are considered null areas and all areas are calculated into polygons. In all polygons, random points are generated and 100 square meter plots are created at these points to assess the vegetation using modified Daubenmire plots. Big sagebrush was the dominant shrub in the overstory of both occupied and unoccupied territories. Annual grasses, annual forbs, litter and bare ground in the understory varied greatly between occupied and unoccupied territories and will be considered significant when developing the HSI model. A suitable habitat model may be created from the data gathered, therefore mitigating any habitat loss or modification.

Developing Micropatterns of Thermoreversible Gels. YOUNG-ME CHUNG (University of California, Berkeley, Berkeley, CA 94720) BARBARA TARASEVICH (Pacific Northwest National Laboratory, Richland, WA 99352).

Biocompatible materials organized into micropatterns have several potential high-throughput screening applications: cell arrays, protein arrays, pharmaceutical assays, and environmental biosensors. Micropatterns of thermoreversible gels have the advantage of providing a biocompatible, hydrating, three-dimensional environment that can sustain the biological functions of specimens such as proteins and cells, both of which can be seeded into or placed on top of the micropatterned gels. We attempted to develop a reliable procedure based on soft lithography techniques to micropattern the thermoreversible gels, N-isopropyl acrylamide (NiPAAm) and collagen. Micropatterns with dimensions ranging from 100 to 1000 microns were obtained with varying success and characterized by optical microscopy in a dried state. Further work to develop a procedure yielding increased success and reproducibility in gel micropatterns is needed. Eventually, hydrated gel micropatterns may be imaged and collaborations to study cell growth or tissue engineering using the thermoreversible gel micropatterns may take place.

Effect of Surfactant Choice on Citric Acid Fermentations using the Fungus *Aspergillus Niger*. LAURA HUBBARD (Walla Walla College, Walla Walla, WA 99362) ROBERT ROMINE (Pacific Northwest National Laboratory, Richland, WA 99352).

Optimization of fungal bioprocess can be impacted by how spores are harvested from the inoculum. The type of surfactant used to harvest spores can influence the efficiency and ease of spore harvest and ultimately impact the production of the metabolites of interest. Understanding impacts that these surfactants have on a fermentation allows for finer control of the fermentation. This paper explores three different surfactants: Triton X-100, a polyoxyethylated octyl phenol commonly used for cleaning osmosis membranes; Span-80, a hydrophobic surfactant that is based on the sugar alcohol sorbitol and contains an 18 carbon chain; and Tween-80, the traditional harvesting surfactant which is also based on sorbitol and is a polyoxyethylene derivative. The main concern of this study is each surfactant's effect on viability, morphology

and conversion of glucose to citric acid (CA) in the fungus *Aspergillus niger*. Triton X-100 averaged a yield similar to the average yield of Tween 80 but was easier to use and produced a much more desirable morphology.

Evaluating Post PIT Tagging Survival and Tag Retention in Juvenile Fall Chinook Salmon. ADAM SEALOCK (Washington State University, Pullman, WA 99163) GEOFFREY MCMICHAEL (Pacific Northwest National Laboratory, Richland, WA 99352).

A passive integrated transponder, or PIT tag, consists of an antenna and circuit encased in glass. To estimate survival through parts of the Columbia basin, the tags are injected into the body cavities of hundreds of thousands of salmonids annually. A total of 80,000 hatchery subyearling fall chinook salmon from the Priest Rapids Hatchery were PIT tagged beginning May 27 and ending May 31, 2003. PIT tags were removed from all recovered mortalities and shed tags were recovered from the bottom of each raceway. Fish length data was used to determine whether there was a relationship between the subyearling fall chinook salmon that died and shed tags when compared against the total tagged population. A total of 294 post-tagging mortalities and 120 shed tags were analyzed. A t-test showed that PIT tag mortalities were significantly shorter ($p = 0.00003$) than the tagged fish population. Another t-test showed that fish that shed their tags were significantly shorter ($p < 0.001$) than the tagged fish population.

Fluorometric Assay Optimization using *Shewanella oneidensis* MR-1. MARIE FORSYTHE (WSU Tri-Cities, Richland, WA 99352) MARGARET ROMINE (Pacific Northwest National Laboratory, Richland, WA 99352).

Shewanella oneidensis is a remarkable bacterium that has the ability to respire heavy metals and transform them from a soluble to a precipitate form. It also has the ability to live aerobically or anaerobically. With such diverse capabilities, *S. oneidensis* is being studied at Pacific Northwest National Laboratory under the Microbial Cell Project as a potential biological remedy to the Department of Energy sites contaminated during nuclear weapon production. Approximately 60 different GFP (green fluorescent protein) promoter-reporter plasmids of *S. oneidensis* have been previously constructed. The goal of this project was to construct new promoter constructs and optimize a fluorometric assay to more efficiently study the expression levels of GFP from these constructs under various growth conditions. Potential clones have been identified; however further screening will be performed to confirm they contain the promoter of interest. Preliminary results from the fluorometric assay suggest that using a protocol with increased shaking time may decrease cell clumping, giving more accurate fluorometric and optical density results. Further research will focus on modifying the protocol to increase the accuracy of this assay. Studies may also be performed on the various constructs by starving the cells of iron using dipyriddy (an iron chelator).

Gene Cloning, Expression, and Purification of Important Proteins from *Pseudomonas aeruginosa*, *Bacillus subtilis*, and *Vibrio cholerae*. BRIANNA KLEIN (University of Oregon, Eugene, OR 97403) MICHAEL KENNEDY (Pacific Northwest National Laboratory, Richland, WA 99352).

Antibiotic resistant pathogens are increasing in number and variety; therefore new antibiotics that target susceptible metabolic pathways or proteins involved in the virulence of pathogenic organisms are needed. *Pseudomonas aeruginosa*, a multi-host human opportunistic pathogen that infects plants, animals, nematodes, and insects, has very specific proteins required for its survival which are good targets for new antibiotics. The mevalonate-independent pathway, in particular ispH and ispG, is not used in vertebrates so antibiotics that directly affect the mevalonate-independent pathway will be effective against pathogens and have low toxicity levels for humans. Determination, by X-ray crystallography, of the three-dimensional structures, of each of these proteins used for pathogenic survival or virulence, will make it feasible to create antibiotics that fit the protein structure. To create good crystals for diffraction, the process of expressing proteins was optimized. The proteins were cloned into pET vectors and expressed using *E. coli* expression hosts. The proteins were isolated and purified using metal-affinity columns with a variety of buffers, concentrated, and crystal trials were prepared. There was not enough protein purified for the majority of the *Pseudomonas aeruginosa* genes to run crystal trials, because of difficulty in purification process. Further purification steps, such as refolding, are needed prior to crystal formation for these proteins. One of the *Pseudomonas aeruginosa* genes, a multiple virulence factor Regulator, was purified and set up in crystal trials at a low concentration. The ispH protein purified from *Bacillus subtilis*, and the ispG protein isolated from *Vibrio cholerae* were also prepared for crystallization, but at higher concentration for crystal trials. At the time of this paper, no crystals have

formed in the crystal trials. It is a strong possibility that in the following months crystals will form and be used for three-dimensional structure determination.

Identification of Landscape Indicators for Sustainable Community Development. JACOB GARZA (*University of Texas at San Antonio, San Antonio, Texas 78249*) KIM M. FOWLER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Indicators are widely used to measure where a system is headed, where it is, where it wants to be, and how it can get there. This paper discusses the use of landscape indicators to measure the environmental, societal, and economic impact of a landscape in the context of sustainable community development. The environmental indicators that determine soil and plant health, and the amount of material/energy inputs a landscape receives and societal indicators that include the number of sustainable landscapes in use or development per square mile and opinion scores that rate public opinion on the aesthetics, functionality of the landscape, and the amount of time spent on the landscape. Economic indicators include the number of businesses supporting sustainable landscapes, maintenance costs, and first cost/replacement cost comparison.

Investigating Use of Building Energy Simulation Tools Based on Data Collection During the 2002 Solar Decathlon. CORRY HAILEY (*University of Missouri-Rolla, Rolla, MO 65409*) KIM M. FOWLER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Numerous building energy simulation tools are available to support the design of more energy efficient buildings. Due to the recent display of advanced building designs at the Department of Energy's 2002 Solar Decathlon, the question of how well these energy simulation tools address innovative building design has arisen. The Solar Decathlon is a student competition to design and build a 100% solar powered house. Fourteen teams brought their houses to the National Mall during the fall of 2002 to compete in the inaugural event. Each team modeled their house using a simulation tool with the results compiled into a final report for the competition. Data from the Solar Decathlon was used to perform an empirical validation of the simulation tools used. Lack of data from the competition caused the empirical validation to be inconclusive, but other observations were made during the process. It was found that the percentage of total energy consumed by the heating, ventilation, and air conditioning (HVAC) systems in each house was nearly half of the percentage consumed by a typical residential building and that the total energy consumed by each house varied greatly among the teams. A review of the final reports was used to supplement the observations made from the analysis. The similarities found were compiled; they include the difficulties the teams had with the simulation tools, the number of tools each team used, and how the teams were able to use the tools for comparison of materials and systems. This paper describes the challenges the Solar Decathlon teams had with using building energy simulation tools to model their innovative buildings.

Locating and Characterizing Anuran Breeding Sites. BRIAN MILLER (*Washington State University, Pullman, WA 99163*) BRETT TILLER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Riparian zones are found adjacent to water courses such as streams, rivers, or ponds and represent the interface between terrestrial and aquatic environments [1]. The riparian environments along the Columbia River shoreline at the Hanford site provide potential amphibian breeding sites. Irregular water levels created by Priest Rapids Dam upstream creates shoreline pools that can be utilized by various herpetofauna that exist within the region. The guidelines of this study were to locate and characterize pools within the Hanford Reach that have created acceptable breeding sites for anurans and identify the species that utilize them. Fifteen pools within the Columbia River's riparian zone were located and characterized with three species of anurans found utilizing these pools, the Great Basin Spadefoot (*Spea intermontana*), Woodhouse's Toad (*Bufo woodhousii*), and the Bullfrog (*Rana catesbeiana*). With appropriate data taken at each site, predictions were made about what habitat characteristics were most favorable for various species.

Mapping the Way to a Sustainable Mindset. RUSSELL FREEMAN (*St. Philip's College, San Antonio, TX 78203*) KIM M. FOWLER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The determination of a community's state of mind could serve to facilitate sustainable development. One technique for measuring the mindset is through surveying. Examples of existing surveys include the Ecological Footprint, Citizen Sustainability Assessment, and Community Sustainability Assessment. These surveys were designed to be given independently but could be used together. This tripod method to surveying offers multiple views of a community's mindset on sustainable devel-

opment. This paper briefly describes survey methodology and proposes the tripod method for integrating the three aforementioned surveys.

Method Development: Protein Separation and Identification in SK-OV-3 Cancer Cell Membrane Receptors. JENNIFER EDGAR (*Montana State University, Bozeman, MT 59715*) DEANNA AUBERRY (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Ovarian cancer is a deadly disease that often evades early detection. The cell line SK-OV-3 was isolated from an advanced stage ovarian cancer patient. Identification of specific peptides in SK-OV-3 membrane proteins will further understanding of how these cells propagate in the body, and possibly lead to targeted biomarker tests for better detection. This study sought to validate previous findings on protein separation and optimize identification techniques for future experiments. All proteins have a specific isoelectric point (pI) that is dependent on the number of charges on the protein. The technique of Isoelectric focusing (IEF) was employed to separate complex mixtures of proteins into simpler fractions according to charge (pI). These protein samples were further prepared for identification by proteolytic digest. Considerable (30-40%) volume loss should be expected with the Rotofor system along with loss of protein sample (50-90%). Removal of detergents and ampholytes added in sample preparation must precede Liquid Chromatography/Mass Spectrometry (LC/MS) analysis, and these additives may also affect IEF results and protein assays. This method of protein fractionation is labor-intensive and involves considerable protein loss, so it may be better suited for samples with a large (>2mg) amount of initial protein.

Multi-Beam System: Its Use in the Strobe Light Deterrent Efficacy Test and Fish Behavior Determination at Grand Coulee Dam Third Powerplant Forebay study. CHARLES JOSEPH (*Eastern Washington University, Cheney, WA 99218*) DAN TANO (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Pacific Northwest National Laboratory (PNNL) and the Colville Confederated Tribes (CCT) are conducting a multi-year research study. The research to assess the efficacy of a prototype strobe light system to elicit a negative phototactic response in kokanee salmon (*Oncorhynchus nerka*) and rainbow trout (*O. mykiss*) in the forebay to the third powerplant at Grand Coulee Dam is in its third year. This year is the first in which a multi-beam system was used to determine fish behavior at Grand Coulee. The multibeam data gathered from this year's study will help to determine if fish are moving past the lights outside of the split-beam system's range. This will enhance the ability to see fish behavior in the vicinity of the strobe light system.

Quantifying HER2 Homodimerization in Cultured Cells Overexpressing HER2. GRETCHEN CARR (*Brigham Young University, Provo, UT 84602*) GALYA ORR (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Human epidermal growth factor receptor 2 (HER2) is a member of the epidermal growth factor (EGF) family of tyrosine kinase receptors. Activation of HER2 under normal conditions occurs through dimerization with other members of the EGF family. HER2 has been shown to be the preferred dimerization partner for all EGF family members and these heterodimers are being studied extensively. Less is known about HER2 homodimerization. Overexpression of HER2 occurs in 30% of human breast cancers and is associated with more aggressive clinical behavior. In this work, we use fluorescence lifetime imaging to quantify HER2 homodimerization in cells overexpressing HER2. Fluorescence lifetime imaging is a method of measuring fluorescence resonance energy transfer (FRET) that is not affected by the concentration of the fluorophore. The results of this experiment show both qualitatively and quantitatively that donor and acceptor molecules bound to different HER2 molecules participate in FRET. This indicates that there are HER2 molecules within very close proximity to each other at the cell membrane, and suggests the existence of HER2 homodimers prior to adding EGF to the system. It is possible that HER2 homodimerization is one of the mechanisms that alter the behavior of these cells.

The Migrational Movements of Bull Trout Observed Along the Priest and Pend Oreille Rivers. JOSEPH BALLENGER (*Winthrop University, Rock Hill, SC 29733*) RICHARD S. BROWN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Bull trout (*Salvelinus confluentus*) have become a concern to many fishery scientists since their first designation as a separate species from the Dolly Varden (*S. malma*) in 1978. Their numbers have dwindled to where in 1998 they were designated as 'threatened' by the U.S. Fish and Wildlife Service. Migratory life histories of bull trout are divided between anadromous (marine and freshwater life stages), fluvial (migrate to large rivers), and adfluvial (migrate to lakes) life histories. This study looked at the juvenile and adult migratory movements of bull trout within

the upper Pend Oreille sub-basin, Idaho. The migratory movements of juveniles and adults in the Middle Fork of the East River were observed to determine if individuals migrate into Lake Pend Oreille or if some are entrained below the Albeni Falls Dam. Bull trout were captured through electro fishing and night snorkeling in the Middle Fork of the East River and just downstream of the Albeni Falls Dam. A total of 141 bull trout were captured and 131 were considered juvenile bull trout. Ten adult bull trout were captured below the Albeni Falls Dam. Of the 141 bull trout captured, 140 were pit tagged and 15 ranging in size from 21-44g were tagged with radio transmitters. In addition, seven adult bull trout were tagged with radio transmitters. Also, eight adult bull trout that were tagged with radio transmitters the previous August were tracked. Individuals were tracked by the positioning of several radio transmitter receivers along the 28 mile stretch of Pend Oreille River between Lake Pend Oreille and the Albeni Falls Dam and by individuals tracking from an airplane and from a truck. The adults moved from the Middle Fork of the East River and overwintered either in the Pend Oreille River or Lake Pend Oreille. Three tagged adults were observed moving into the spawning areas the following June and July. No migratory movements were seen in the 15 juveniles after they had been tagged. From the results it is seen that at least some adult bull trout that overwinter in Lake Pend Oreille and the Pend Oreille River migrate to the Middle Fork of the East River to spawn in the fall months. Because of the lack of movement seen in the tagged juveniles no conclusions can be made about what percentage of juveniles migrate upstream into Lake Pend Oreille or down stream past the Albeni Falls Dam.

Understanding Metabolic Pathways of Disinfection By-Products in Rat and Rainbow Trout Liver Tissues. EVAN ADAMS (*Whitman College, Walla Walla, WA 99362*) IRV SCHULTZ (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The process of disinfecting drinking water has saved countless lives since its implementation, however it also creates hazardous by-products. Haloacetic acids (HAAs) are one of these by-products, many of which are labeled as carcinogens. To understand the metabolic processing of chlorodibromoacetate, a HAA, we used rat and rainbow trout liver tissue in a series of in vitro experiments. In these tissues the cytochrome p450 (CYP450) family of enzymes was the primary catalyst of metabolism. Two inhibitors were used to identify the specific CYP450 isoform responsible. In both the rat and trout tissues sulphenazole, a CYP2A1 inhibitor, had no negative effects on total metabolism while ketoconazole, a CYP2E1 inhibitor, had a very large negative effect. The CYP450 isoform that metabolizes HAAs in rats is probably the same in humans, rats have historically been used in toxicology and human health experiments. Interestingly, the trout tissue mirrored the results of the rat tissue. Trout have never been accepted as a toxicological model, but it appears that in this case they might be useful as an alternative model species in future studies of disinfection by-products.

Wastewater Treatment and Technology for Sustainable Community Development. AMY SCHNEIDER (*University of Missouri-Rolla, Rolla, MO 65409*) KIM M. FOWLER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

This paper presents wastewater treatment options that can satisfy a community's needs in an effective and sustainable manner. By performing an analytical review of current wastewater trends, we found a disconnection between current wastewater trends and sustainability. Wastewater treatment is a concern for communities because the cost of treating the nation's wastewater is huge and rapidly increasing (GAO, 1994), and because of its dependence on high quality and quantity of water. We summarize principles for water and wastewater management, wastewater treatment options, and social, economical, environmental and technical considerations that need to be part of wastewater planning. The paper also provides a list of useful tools and resources.

CHEMISTRY

Analysis of the Use of Magnesium Oxide, Calcium Oxide and Sodium Hydroxide for the Solidification of Uranyl Nitrate Solutions for Storage. KRISTINA FELFE (*Illinois Institute of Technology, Chicago, IL 60616*) CALVIN MORGAN (*Argonne National Laboratory, Argonne, IL 60439*).

The hot cell wing of the analytical laboratory at Argonne National Lab - West regularly receives samples to analyze, many of which contain uranium compounds and must be dissolved in nitric acid for analysis. When the sample is dissolved in nitric acid, a solution of uranyl nitrate, $UO_2(NO_3)_2$, is formed. Only 5-10% of the solution is used for analysis and the remainder of the solution must be consolidated with other solutions and solidified to be put into storage. The solid must meet a "no free liquids" criteria and also must have a pH between 5 and 11.

The ease of the procedure and ease of removal of the solid were also considered. This paper covers the study of ten different methods of solidifying a surrogate uranyl nitrate solution using MgO, CaO and NaOH. The different methods that were used included evaporating the solution to dryness and adding the reactant; evaporating the solution to dryness, dissolving the solid and adding the reactant; and decreasing the volume of the solution and then adding the reactant. It was found that the use of NaOH resulted in pH values that were much too high. Reducing the volume but not evaporating the solution to dryness was determined to result in the release of a large amount of heat upon the addition of the oxide. The optimal method was found to be evaporating the solution to dryness and dissolving the solid in a minimal amount of water. Then adding MgO in a 4:1, MgO: $UO_2(NO_3)_2$, ratio. This method resulted in a solid that met all the regulatory requirements and the procedure was also easy to carry out, making it optimal for use within the analytical laboratory hot cells.

Analytical Chemistry: A Review of the Analytical Lab. EARLE WOLFROM (*The Evergreen State College, Olympia, WA 98505*) MARSHA LAMBREGTS (*Argonne National Laboratory, Argonne, IL 60439*).

Analytical chemistry at Argonne National Laboratory - West is an integral part to most all of the facilities at the Eastern Idaho site. The understanding of the instruments by those submitting samples was deemed insufficient. This paper describes the Analytical Laboratory at Argonne National Laboratory - West, the methods applied, and theories of the instrumentation. The facility supports many ongoing processes for the many facilities and is important for the future of nuclear energy.

Characterization of Plutonium Oxide by Micro-Column Extraction and Inductively Coupled Plasma Mass Spectroscopic (ICP-MS) Detection. BRANDON MCALLISTER (*Albertson College of Idaho, Caldwell, ID 83605*) DAN G. CUMMINGS (*Argonne National Laboratory, Argonne, IL 60439*).

Reprocessed, reactor grade plutonium fuels require the quantitative determination of actinide and metal components to guarantee the efficiency and purity of reprocessing. Analyses of plutonium oxide (PuO_2) by ICP-MS are complicated by isobaric interferences, and instrumental considerations. Herein a method to detect trace levels of actinides (Pu, U, and Am) and a variety of trace metals of interest are reported. The process utilizes a novel gas pressurized extraction system with commercially available TEVA[®] resin to remove Pu from the matrix, thus avoiding isobaric interferences for other actinide determinations. The Pu is then recovered from the resin material and analyzed. The micro-column volume was approximately 35 μ L, while utilizing approximately 77 mg of resin material. Separation efficiencies measured by ICP-MS for U and Am are 100 %, while Pu is on the order of 99.5 %. Standard deviations are on the order of 1%. The ability of the TEVA[®] resin to perform trace metal analyses in a Pu matrix was also tested with a variety of metals. Recoveries for greater than 30 metals through the analytical column ranged between 100 -103 % recovery, at the low ng/mL range. Additionally, modifications to instrument hardware and the use of optima grade solutions allowed for trace level detections of Boron (B) in the PuO_2 matrix. Instrument detection limits for B were on the order of 70 pg/mL, with analytical sample spike recoveries of 104 %. Thus, an analytical method for ICP-MS has been developed to characterize the PuO_2 sample for trace metal content as well as actinide content in a single separation.

Corrosion of Nickel Based Superalloys Exposed to Ash Conditions Similar to Those in Coal-fired Power Plants. STACY GRANT (*Schenectady County Community College, Schenectady, NY 12306*) ANKUR PUROHIT (*Argonne National Laboratory, Argonne, IL 60439*).

Coal-fired power plants are responsible for 51.4% of total electricity generated in the US. The power plants and metal parts within are very susceptible to corrosion. The high temperatures and compositions of the coal and ash byproducts are highly corrosive. 1x3 cm sized pieces of Inconel 600, Haynes 214 and Haynes 230 were cut from rolled sheet stock and were then covered in loose ash. Ash #1 consisted of 30.00g Al_2O_3 , 30.00g SiO_2 , 30.00g Fe_2O_3 , 5.000g Na_2SO_4 , and 5.000g K_2SO_4 and ash #3 consisted of 29.25g Al_2O_3 , 29.25g SiO_2 , 29.25g Fe_2O_3 , 5.625g Na_2SO_4 , 5.625g K_2SO_4 , and 1.000g NaCl. The samples were [placed in horizontal tube furnaces supplied with laboratory air mixed with 1% (by weight) SO_3 . The temperature was set at 650° C, 725° C and 800° C. At various time intervals the samples were removed, weighed and the oxide layers collected. After 336 hours at 800° C all alloys showed significant corrosion and disintegrated by 504 hours. After 168 hours at 725° C all alloys showed some forms of corrosion. At this time no conclusions can be made as the tests are ongoing and further analysis is required.

Fluorescence Polarization. MICHELLE GREIGG (*Miami-Dade College, Miami, FL 33132*) ISTVAN NADAY (*Argonne National Laboratory, Argonne, IL 60439*).

Fluorescence Polarization (FP) enables researchers to view molecular binding events in solution. Design engineers are seeking to develop a miniature, field-useable instrument to detect specific target molecules (antibodies), such as Anthrax or Tuberculosis, in saliva samples. Fluorescently labeled molecules are added to the sample. These special molecules have two unique properties: (i) they emit light with some time delay at a different wavelength but same polarization as that of their illumination and (ii) they bind to specific target molecules, if present. If these fluorescent molecules do not find large target molecules, due to their small size they rotate and move quickly from one plane (excitation) to the next (emission). Therefore the polarization of the emitted light will not be connected to the polarization direction of the excitation. However, if these special molecules find the target molecules, they bind, and their volume increases thus decreasing their rate of rotation. Consequently, the emitted light will have the same polarization as the excitation light. Once we illuminate the sample using a single wavelength of polarized light, we measure the response of the emitted light in two polarized planes, the horizontal and the vertical. If we find that the emitted light has the same polarization as that of the excitation, we can be sure that the small molecules are connected to large target molecules through their slow rotational spin. This indicates the presence of such antibodies. If the emitted light has no polarization (vertical and horizontal are similar), this means that the small free molecules rotated quickly and did not detect the large target molecules, so that sample does not contain the target material.

Inert Anode for Aluminum Production. ANTHONY FITCH (*University of Nebraska - Kearney, Kearney, NE 68849*) JIANHONG YANG (*Argonne National Laboratory, Argonne, IL 60439*).

In 1886 Hall and Heroult developed an electrolysis process to obtain aluminum metal from alumina. Since then researchers have been working on ways to decrease the energy consumption of aluminum electrolysis and reduce the release of greenhouse gases. However, most of the resources have been exhausted for this specific process. The goal of this project is to find an inert alloy to replace the currently used carbon anode. This would result in reduced greenhouse gases and lower energy consumption. Different alloys have been tested using a low temperature electrolyte in a smaller cell for 24 hours and at 10amps. The small cells have produced 50% to 60% current efficiencies. The aluminum was then dissolved and analyzed by Flame AAS for certain metals. One sample was found to be 0.706% Cu, 0.044% Fe, 0.028% Ni, 0.241% K. The more promising alloys were then used in a larger cell to run for 100 hours at 100amps. Alumina was feed into the cell during electrolysis and more than a kilogram of aluminum has been produced. However none of the alloys have lasted the full 100 hours. The longest one made it a little more than 90 hours, but suffered severe corrosion. The aluminum collected from the larger cell contained high percentages of impurities due to the corrosion of the anode. Once a suitable alloy has been found it will be tested on a pilot plant and then in an industrial plant.

Modeling Vibronic Spectra of Heavy Elements in Solids. KENT SCHONERT (*Illinois State University, Normal, IL 61761*) GUOKUI LIU (*Argonne National Laboratory, Argonne, IL 60439*).

Actinides and lanthanides doped in glass and crystal lattices often have strong electron-phonon coupling, which influences their fluorescent spectra in unique ways. A strong electron-phonon coupling results in changes in lattice equilibrium positions, electric dipole moment, and vibrational frequencies during their transition between electronic states. The theoretical model for these spectra utilizes a large number of parameters. For many of these parameters only the ranges or approximate values are known. By fitting data from experimental spectra using a model developed by G. K. Liu et al. [1], it is possible to extract information about the characteristics of the structures and electronic properties of these heavy elements in solids. Using the Levenberg-Marquardt numerical technique, optimized parameters often can be found efficiently for the computational model of these spectra. While a C++ written console application runs the calculation of the model and the optimization of its parameters on the back-end, the front-end Graphics User Interface, written in Microsoft Visual Basic, provides a user-friendly environment for the input of parameters, model settings, and implementation of save/load features. This combination of user-friendly environment coupled with efficient numerical techniques may be a promising tool for scientists in the fields of inorganic chemistry and condensed matter physics.

Modifications of an STA 409 PC In Order To Obtain More Accurate Results For Analysis. JACKLYN GATES (*Westminster College, New Wilmington, PA 16172*) J. RORY KENNEDY (*Argonne National Laboratory, Argonne, IL 60439*).

As part of the Advanced Fuel Cycle Initiative (AFCI) program, non-ferri- plutonium-zirconium (Pu-Zr) based alloys, with additions of uranium (U), americium (Am) and neptunium (Np), have been cast using an arc-melting process. These alloys are being irradiated in the Advance Test Reactor (ATR) to evaluate their possible use for transmuting long-lived transuranic actinide isotopes. The as-cast alloys have been measured for their thermal characteristics using Differential Thermal Analysis/ Differential Scanning Calorimetry/ Thermogravimetric Analysis (DTA/DSC/ TGA) up to 1000°C. However, initial analysis of the alloys highlighted several difficulties in obtaining accurate measurements, namely oxidation of alloys, calculations resulting in negative heat capacities and lack of reproducibility of results. These difficulties were combated via modifications to the instrument or materials.

New Approaches to High Power Medical Batteries. MARLON HUDSON (*Alabama State University, Montgomery, AL 36601*) JOHN VAUGHEY (*Argonne National Laboratory, Argonne, IL 60439*).

Implanted medical devices powered by electrochemical power sources play a vital role in the treatment of disease and the well-being of patients. The development of the lithium-ion battery is making contributions to producing less expensive medical devices offering good voltage and higher energy capacities. Our goals were to develop and characterize a class of high powered primary or secondary lithium-ion batteries to run the next generation of implanted medical devices. The study evaluated silver polymers as cathode materials in primary lithium-ion batteries. Another area we studied was vanadium polymers as cathode materials in secondary lithium-ion batteries. Materials were tested using a MACCOR Battery Testing controller. Cells were evaluated between 3.5-0 V for the silver compounds, and 4.5-1.0 for the vanadium compounds. A current of 0.1 mA was used for all tests. Future work will focus on biological activity and study materials which mimic insulin.

Primary Light Reactions of Green Plant Photosystem I: Advancing the Technology of Tomorrow. TARRAH MIRUS (*East Carolina University, Greenville, NC 28532*) MARION THURNAUER (*Argonne National Laboratory, Argonne, IL 60439*).

The process of photosynthesis is essential to all living things on earth. As scientists we are interested in this process at many different levels. For example, in order to understand how light energy is converted into chemical energy we must understand the basic electron transfer reactions that take place within a reaction center protein. Photosynthesis begins when a chlorophyll dimer within a reaction center protein is irradiated with light. This dimer (known as the special pair) absorbs the light, thus creating an electronic excited state. This begins an electron transfer (ET) process to two neighboring acceptor molecules, resulting in a charge separation across the membrane that is essential in photochemical energy conversion. Past research has shown that within the reaction center there is a symmetrical structure of molecules (cofactors) composed of the special pair, two neighboring chlorophylls, two pheophytin molecules (in bacterial systems), and at the ends of each branch are quinones. In the Photosystem I (PS I) reaction center there is an iron sulfur complex (Fx) between the two quinones which participates in ET. Research on the bacterial system has been used to help study the more complex green plant photosystems. In a bacterial system ET flows down one branch and moves from one quinone on the structure to the other. PS I has caused much controversy regarding the exact pathways that ET takes due to the fact ET goes directly from one (or both) quinones to Fx. Thus, it is thought that both branches of the cofactors may have the ability to carryout ET all the way through to Fx. The purpose of this project was to study the charge separation between chlorophyll-(P+) and quinone-(Q-) in hopes of discovering the pathways that each electron travels through to create this charge separation. These relationships were studied through the use of time-resolved pulsed electron paramagnetic resonance (EPR). Although the exact ET pathways were not discovered through this experiment, many other interesting anomalies were seen for the first time. The sensitivity of the home built EPR system that was used allowed us for the first time to look more closely at the changing shape of the echo as well as to confirm that PS I signals experience unusual time dependent phase shifts. This experiment poses many future opportunities for further understanding of both PS I and up and coming technologies in pulsed EPR spectrometry.

Sulfur Removal From Reformate. KENDRICK TURNER (*Murray State University, Murray, KY 42071*) XIAOPING WANG (*Argonne National Laboratory, Argonne, IL 60439*).

While the use of fossil fuels is being investigated as a source of hydrogen-rich reformat to be used in fuel cell applications, sulfur content

of these fuels has a poisoning effect of fuel cell components. If fossil fuels are to be used as a hydrogen source for fuel cells, sulfur must be removed to prevent this poisoning effect. The DOE has set a goal of removing sulfur to below 10 ppb by 2010. Materials consisting of transition metal oxides impregnated on a support material are being investigated to reduce the sulfur content in gaseous reformat after reforming but prior to introduction into the fuel cell stack. Several of these materials have been shown to meet the DOE target, and current work focuses on methods of optimizing performance of these sulfur-sorbent materials.

Synthesis & Characterization of Polymer Nanocomposites Used in Lithium-Ion Batteries. MONICA VILLAR (*Pima Community College, Tucson, AZ 85745*) GISELLE SANDI (*Argonne National Laboratory, Argonne, IL 60439*).

Polymer nanocomposites are being studied to find novel ways to replace the liquid electrolytes of lithium-ion batteries. The PNCs are transformed into a solid state in the form of a membrane, or film. These films are said to mimic the properties of the liquid electrolytes, but will be more efficient, have greater storage capacity and simplified manufacturing that lead to convenience and low cost production. The synthesis and characterization is a crucial part in understanding and developing accurate polymer nanocomposites. Utilizing hectorite clays that are intercalated with different mass ratios of poly(ethylene oxide) provide mobility for the lithium cations for conductivity, while mechanical strength is still maintained. Synthetic Lithium Hectorite was the hectorite clay prepared using hydrothermal crystallization for 48 hours. Characterization was done by X-Ray Diffraction, Thermogravimetric Analysis, BET and conductivity tests. An XRD inset of PEO/SLH membrane indicates the diffraction peaks of PEO intercalated into the clay galleries. TGA was used for comparative purposes for the actual versus the theoretical ratios of PEO and SLH. BET measured a surface area of 229.7 m²/g and an approximate pore diameter of 20 Å. Conductivities range from 1-2 x 10⁻⁵ Ω/cm, which is very good considering it is a solid material. As expected, when the temperature is increased, the conductivities also increased. Future work includes studies at the Advanced Photon Source for small-angle X-ray scattering studies, transference number determination, preparation of polymer membranes of different molecular weights, and film spectroscopy of characterization.

Synthesis and Evaluation of Layered Oxide Anodes and Cathodes for Lithium Ion Batteries. ANDREA DAWSON (*DePauw University, Greencastle, IN 46135*) JOHN VAUGHEY (*Argonne National Laboratory, Argonne, IL 60439*).

Since the introduction of the lithium battery by Sony in 1990, there has been a revolution in the consumer-based electronics industry. Current research focuses on developing cheaper, safer, and less toxic battery materials. In response to the need for safer batteries, several layered cathodes and anodes of the formula Li₃MO_b (M= Mo, Mn, Zr, Pr, Ti) and XMTiO₄ (X=Li, Na; M= La, Pr) were synthesized using high temperature and molten lithium ion exchange methods. The synthesized lanthanide and transition metal based materials were characterized using powder X-ray diffraction and electrochemical methods. The developed materials were analyzed electrochemically with respect to lithium to determine their feasibility in lithium ion batteries and their properties. Electrochemical studies indicated that Li₂MO₃ (M = Mn, Mo) adopted a classical insertion mechanism with as many as 2 lithiums inserted per formula unit. On the other hand, the Dion-Jacobson intercalation materials only displayed a lithium insertion of 0.5, most likely due to a structural limitation in the materials. Similar capacities (approx. 50 mAh/g) were achieved from the related compounds LiPrO₂, Li₂ZrO₃, and Li₂TiO₃. The compound LiMoO₂ shows promise as a cathode, with a relatively high capacity (199 mAh/g) and voltage (3.0 V) being achieved relative to LiCoO₂/graphite cells.

Synthesis of Magnetic Nanospheres and Microspheres for Controlled Drug Delivery System and Toxin Removal. ADETOWUN ALIMI (*Maloclom X College, Chicago, IL 60612*) KAMINSKI, MICHAEL (*Argonne National Laboratory, Argonne, IL 60439*).

Magnetic microspheres and nanospheres for controlled drug delivery system and for toxin removal of radionuclides. Low level of drug can be sub-therapeutic and high level can cause toxicity or even death. Targeted drug delivery system may result in lowering of adverse toxic effects and enhancement of therapeutic efficacy. The ultimate goal of drug delivery is the ability to incorporate drugs without damaging them, release of drugs at its target location such as cells and tissue and ability to be retained in the system without being recognized as a foreign object by the immune system. Poly Ethylene Glycol polymers are known and widely used for coating due to high biocompatibility and antiposonizing effect. PEG polymer has an adsorption surface layer, which forms a hydrophilic barrier. Polymers can also be used as stabilizer of colloidal dispersion due to their surface coating of metastable microspheres,

which lowers surface aggregation. These magnetic microspheres will be intravenously injected into human body, and maneuvered using ultrasound to specified target cell or tissue locations as needed. These magnetic nanospheres will also be injected into the human body intravenously but the will be used to remove specific toxins such as cesium or any other toxins they are designed for. The microspheres will contain drug such as T- Plasminogen A (tPA) a pharmaceutical drug used to open blood clots in the brain.

Testing Novel Additives for Lithium-Ion Battery Electrolytes. MONIQUE DIAZ (*Pomona College, Claremont, CA 91711*) YOO EUP HYUNG (*Argonne National Laboratory, Argonne, IL 60439*).

Lithium batteries produce current by shuttling lithium ions between the anode and cathode, causing electrons from the source of positive ions to accompany them to their destination in order to balance charge. Integral to the movement of lithium ions is an electrolyte that is compatible with the anode/cathode system. The following report is focused on determining which electrolyte and additive combination generates the best voltage window, shelf-life, and is thermally stable. Thus far, results from over one hundred charge and discharge cycles of coin cell lithium batteries have shown that the additives 2% vinyl ethylene carbonate with 1% 2,3-dimethyl-1,3-butadiene, and 4-phenyl-1,3-dioxolan-2-one in 1.2M LiPF₆ carbonate electrolytes dramatically increase capacitance values.

TGA (Thermo Gravimetric Analyzer) Analysis of UH₃. SHARHONDA BUIE (*Alcorn State University, Lorman, MS 39096*) RORY KENNEDY (*Argonne National Laboratory, Argonne, IL 60439*).

The corrosion and oxidation of materials is a major concern in many industries, since it affects the operating lifetime of any number of societal necessities from bridges and buildings to instruments and machines to tools and utensils. In order to develop a better knowledge of corrosion and oxidation, studies were conducted on the kinetics of oxidation of UH₃ (Uranium Hydride) with air. Corrosion of uranium in air at conditions involving fire and humidity is of special concern because the oxidation rate of uranium is dependent on temperature and humidity. The data was collected and analyzed using a thermo gravimetric analyzer (TGA) and the mass/time/temperature relations were analyzed in a variety of ways to develop a model of the reactions. The TGA instrument is able to apply the measurements of absorbed water of crystallization and studies of the thermal stability of substances and decompositions and oxidation reactions from solid to gas to gas to solid. The data was then analyzed using physics and graphing based program called Origin.

The Manufacture of Nondestructive Assay Standards for Uranium Gamma-Ray Spectroscopy. KATHERINE TRAYNOR (*University of Notre Dame, Notre Dame, IN 46556*) ANDREW MADDISON (*Argonne National Laboratory, Argonne, IL 60439*).

The goal of my project was to aid in the development of nondestructive assay (NDA) standards. Epoxy has shown potential to hold uranium, and therefore be used as a method for preparing standards and possibly aid in waste disposal. I observed the behavior of the epoxy in casting it alone and then added an organic solvent to the epoxy during the casting process. Work was done first with a cerium surrogate, and then experimentation with depleted uranium was completed. The epoxy successfully held a sufficient amount of tributyl phosphate, which can eventually be used to extract the highly-enriched uranium (HEU), and mix the organic extractant into the epoxy. Analysis with XRF has shown that the cerium surrogate can be distributed evenly throughout the epoxy, giving much promise for the future attempt at attaining a uniform distribution of uranium in the epoxy.

Development of a Measurement Technique of Atmospheric Ammonia. TRACEY EVANS (*State University of New York Old Westbury, Old Westbury, N.Y. 11568*) JUDITH LLOYD (*Brookhaven National Laboratory, Upton, NY 11973*).

Due to the harmful effects of ammonia on the health of animals including humans and on environmental conditions in the U.S. the scientific community has been moved to take actions into finding ways to detect and contend with it. The investigation described is a study of the effects of changing variables of concentrations, pH, and percentage composition of reagents used in an atmospheric ammonia measurement technique. The apparatus used is a spectrofluorescence detector (McPherson FL-750), with tubing connected to a peristaltic pump pulling (Master Flex) a combination of o-phthaldialdehyde, sulfite reagent containing phosphate buffer, and liquid ammonium. The OPA, sulfite, phosphate and ammonium were changed from there standard to find the sensitivity and parameter that the spectrofluorescence detector best operates under. The resulting finding showed that OPA produced high-quality fluorescence intensities under greater concentrations, with a 12% presence in composition of ethanol; sulfite optimum concentration

was .004M; phosphate best pH was 10.5, with improved results with additional concentration presence; and OPA to sulfite presence percentage being at a fifty-fifty state. Ammonia calibration showed the expected results of as concentration was increased so was fluorescence intensity. Due to these results new parameters were put in place to conduct gas phase detection of ammonia which are producing results in the laboratory at this time and it hoped that future field testing will occur.

LENS, Low-Energy Neutrino Spectrometer - Chemical Analysis. MARY KIDD (Tennessee Technological University, Cookeville, TN 38505) MINFANG YE (Brookhaven National Laboratory, Upton, NY 11973).

In excess of 99% of the solar neutrino flux is at energies below about 1 MeV. The Low-Energy Neutrino Spectrometer (LENS) will attempt to measure the lowest energy solar neutrinos in real-time. LENS will use the neutrino capture reaction in ^{115}In which leads to the prompt emission of an electron and a delayed cascade of two gamma rays. Looking for these three events in coincidence provides a specific signature for the neutrino interaction and helps filter background radiation. The medium in which these reactions take place will consist of an organic liquid scintillator, pseudocumene (PC) loaded with Indium (In-LS). Synthesis methods to prepare In-LS have been developed at Brookhaven National Laboratory (BNL) and other institutes within the LENS collaboration. The chemical properties and light yield of this medium must be assessed before using it as a neutrino detector. The interacting mechanisms by which LENS detects neutrinos as well as the determination of chemical properties, stability, and light yield will be discussed.

The Effect of Ether Functionalities on the Properties of Pyrrolidinium Ionic Liquids. ELINA TROFIMOVSKY (Brooklyn College, City University of New York Honors College, Brooklyn, NY 11214) JAMES WISHART (Brookhaven National Laboratory, Upton, NY 11973).

The term "ionic liquid" refers to a novel class of molten salts that are liquid at ambient temperatures. Ionic liquids hold promise as reaction media with significant economic, environmental, and safety advantages over commonly-used organic solvents. In the design of ionic liquids, lower viscosities are desirable for speedy, efficient reactions and better handling properties for industrial applications. The purpose of the research project was to find out whether the replacement of alkyl groups by ethers would lower the melting points and viscosities of the pyrrolidinium-based salts. To this end, a number of novel pyrrolidinium ionic liquids were synthesized and characterized. Above all, the incorporation of an ether (ROR) branch proved successful in producing advantageously lower melting points and viscosities. Further work to be carried out on these pyrrolidinium complexes will include pulse radiolysis kinetics measurements and solvation dynamics studies using fluorescent probe molecules. The latter investigations will offer insight into the reactivity of solvated electrons and other species in these new media. The new ionic liquids demonstrate a subtle but effective method to control viscosity that will be useful in the effort to understand the process of electron diffusion in ionic solvents, which previous measurements indicate to be substantially slower than in molecular solvents.

The Reduction of Quinones by Cobaltacene. DEVON PONDS (Texas Southern University, Houston, TX 77021) JOHN MILLER (Brookhaven National Laboratory, Upton, NY 11973).

The electrochemical behavior of quinone compounds has been extensively studied, because of their ability to transport electrons and protons in biological processes such as photosynthesis and bacterial respiration. This study is an attempt to test solvent polarities effect, quantity of ion produced and the stability of multiple quinones negative ions with various redox potentials using the reducing agent Cobaltacene CoCp_2 at room temperature. Duroquinone (DQ), Benzoquinone (BQ), 1,4-Napthaquinone, 2-Methyl-antraquinone (2MAQ), Anthraquinone (AQ), 2-Methyl-1,4-napthaquinone, 2-Phenyl-1,4-benzoquinone, 2,5-Di(tert)butyl-1,4-benzoquinone, 2,6-Di(tert)butyl-1,4-benzoquinone, 2,5-Diphenylbenzoquinone, 2,3 Dichloro-5,6-dicyanobenzoquinone, Fluoronile (F \cdot BQ), and Ethylanthraquinone were made into solutions in Tetrahydrofuran (THF) and Methylcyanide (MeCN) and reduced by cobaltacene in 200ml cells. DQ, BQ and F \cdot BQ were reduced quantitatively and BQ, MAQ, and F \cdot BQ were reduced in both THF and MeCN. The quinones were measured using UV/Vis/NIR spectrophotography and solutions were analyzed using IGOR Pro (Wave Metrics). All of the quinones were reduced except AQ. CoCp_2 did not quantitatively reduce DQ and BQ in THF solutions and when MAQ was tested in THF anion was not formed but in MeCN the negative ion was formed. The redox potentials of the quinones as well as the polarity of the solvent are a major factors in the behavior of their reduction by CoCp_2 .

Toluene-induced Conditioned Place Preference in Rats. JUZER TAIBALI (Harry Truman College, Chicago, IL 60660) MADINA GERA-SIMOV (Brookhaven National Laboratory, Upton, NY 11973).

The abuse potential of toluene was investigated in rats using the conditioned place preference paradigm. Sixteen male rats were used for this experiment. Eight rats (control group) were alternatively paired with only air in either the black/the white box for sixteen days. Simultaneously half of the eight rats (test group) were alternatively paired with toluene at 5000 parts per million (8 days) in the white box, and air in the black box (8 days). The other four rats were paired with toluene in the black box (8 days), and only air in the white box (8 days) for the same number of days. Forty-eight hours after the last exposure to toluene, the rats were tested in a drug-free state (without any exposure to toluene) for a conditioned place preference. Naïve rats (control group) showed no preference to either side (black/white box) of the chamber. They have spent approximately equal time on each side (4.03 + 0.56 and 3.9 + 0.57). But the test rats demonstrated statistically significant ($p < 0.01$) preference to the toluene-paired side (5.11 + 0.49 and 3.84 + 0.32). The results indicated that the rats had associated inhalation of toluene with environmental cues. Moreover, toluene, one of the most abused inhalant, elicited positive reinforcement as evidenced by significant increase of time spent on toluene-paired side.

X-Ray Study of Molybdenum Sulfide Nanoparticles. CHRIS VARNNEY (Northern Arizona University, Flagstaff, AZ 86011) MICHAEL WHITE (Brookhaven National Laboratory, Upton, NY 11973).

Molybdenum sulfide is of interest in catalysis because of its high reactivity and is used in several catalytic applications, including photooxidation of organic chemicals and hydrodesulfurization of crude oil. The purpose of this study was to characterize molybdenum sulfide nanoparticles of varying sizes and methods of synthesis. Nanoparticles were synthesized via reverse microemulsions formulated with bis(2-ethylhexyl)sulfosuccinate (AOT) and via sonication of molybdenum hexacarbonyl and of ammonium tetrathiomolybdate (ATTM). Particle characterization was accomplished by Ultraviolet/Visible absorption spectroscopy, dynamic light scattering, and X-ray absorption spectroscopy (XAS). XAS analysis showed that the oxidation number for nanoparticles generated from Mo(CO)_6 sonication is consistent with 5. Furthermore, it was found that there was correlation between the coordination numbers of Mo-S and Mo-Mo bonds and sonication time, attributed to the combination of the cluster size effects and enhanced bond length disorder. XAS measurements for sonicated ATTM and AOT-based microemulsions were not completed at the time of this writing.

Synthesis and Radiolysis of Tertiary Alkyl Ammonium Bis(trifluoromethanesulfonyl)imide Ionic Liquids. RABINDRA RAMKIRATH (Queens College of the City of New York, Flushing, NY 11367) JAMES WISHART (Brookhaven National Laboratory, Upton, NY 11973).

Ionic Liquids (ILs) are salts that are liquid over a wide temperature range. Due to their increasing importance, it is necessary to learn about how chemical reactions occur in these ILs and how the liquids are affected by ionizing radiation. The objective of this study is to synthesize and characterize the family of tertiary alkyl ammonium bis(trifluoromethanesulfonyl)imide, $[\text{R}_3\text{NH}][(\text{SO}_2\text{CF}_3)_2\text{N}]$, ionic liquids, where R = methyl, ethyl, propyl and butyl groups. After synthesizing these ILs, preliminary rates of chemical reactions and chemical reaction mechanisms were investigated using pulse radiolysis. These liquids or low melting solids varied in melting point, viscosity, and solvating power; properties that affect their suitability for chemical kinetics studies. Some other physical measurements reported here are density and refractive index for (N222)(NTf2), the only liquid observed among the family. The liquids with low melting points will be used to study H-atom reactions by pulse radiolysis, and viscosity differences between solvents will be used to examine the mechanism of conversion of electrons into H-atoms.

Evaluation of the Movement of Sodium Phosphate Through a Sili-con Oxide Matrix Using Thin Layer Chromatography Coupled with Secondary Ion Mass Spectrometry. ANGELA CARUSO (Clemson University, Clemson, SC 29634) ANTHONY D. APPELHANS (Idaho National Engineering & Environmental Laboratory, Idaho Falls, ID 83415). Potential migration of subsurface contaminants into the underlying aquifer is a concern at the Idaho National Engineering and Environmental Laboratory. One approach to attenuate migration would be to create a calcium phosphate barrier. To do this, it might be possible to serially infuse the subsurface with soluble phosphate and then calcium to form a precipitate barrier. Thus, the migration of soluble phosphate and calcium through mineral oxide matrices must be understood. In the present study, Thin Layer Chromatography (TLC) and Secondary Ion Mass Spectrometry (SIMS) are used to investigate the mobility of soluble phosphate. TLC plates were used to measure mobility, and SIMS analysis of the developed plates tracked phosphate mobility. In

SIMS, a sample removed from a developed TLC plate was bombarded by energetic ions that disrupted the surface and caused fragments of molecules on the surface to be sputtered into the gas phase, where they are sorted by mass and detected. The resulting mass spectra were correlated with the phosphate species under investigation. The extent of mobility was assessed, and rates of solvent flow as a function of the solute were measured. Our results showed the solute slowed the rate of aqueous infiltration through cellulose and silica matrices. Rate of infiltration decreased in the order: water >calcium nitrate >sodium phosphate. In addition, three different sodium phosphate species were evaluated, and the rate of infiltration was found to decrease in the order: $\text{NaH}_2\text{PO}_4 > \text{Na}_2\text{HPO}_4 > \text{Na}_3\text{PO}_4$. Phosphate displayed a broad, regular distribution with retention factors from about 0.3 to 0.8. In contrast, sodium displayed a bimodal distribution, with an abundant peak at $R_f \sim 0.3$, and a faster moving, broad distribution that ranged from 0.3 to 0.8. These observations show that phosphate and a fraction of the sodium could be moved at a fast rate through the matrix, but a second fraction of the sodium was more strongly retained. SIMS detection limits of sodium on the TLC plates was also evaluated. The abundance of Na^+ increased nearly linearly with increasing concentration from 0.038mM to 2.5M Na_3PO_4 . Above 2.5M, Na^+ abundance did not increase, indicating surface saturation above this concentration. The results indicated that soluble phosphate could be readily moved through the silica matrix, which might enable barrier formation by subsequent infusion of calcium phosphate. This latter experiment is the next stage for this research.

Functional Groups of Soil Bacteria: An Exploratory Study By Sum Frequency Generation (SFG) Vibrational Spectroscopy. JULIA CHAMBERLAIN (Reed College, Portland, OR 97202) HEINO NITSCHKE (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Microbial activity in soils and sediments can significantly affect transport of radionuclides in the environment. A mechanistic understanding of actinide-bacterial interactions, including surface complexation and reduction, is necessary for designing bioremediation methods for hazardous nuclear waste. The most promising new technique for studying biological surfaces and interfaces is Sum Frequency Generation (SFG) spectroscopy. SFG is a highly surface specific non-linear optical process used to study vibrational modes of surfaces and interfaces. In this study, we use SFG to identify surface functional groups of the common soil bacteria *Deinococcus radiodurans* and *Shewanella putrefaciens*. *D. radiodurans* and *S. putrefaciens* were cultured to stationary phase. FTIR and SFG spectra were obtained between 2800-3050 cm^{-1} . FTIR spectra showed the presence of methyl and methylene stretches for the bulk bacteria, whereas the SFG results showed only the methyl stretches on the bacteria surface for both bacterial species. These results suggest the presence of methyl and the absence of methylene groups on the cell surface, but more importantly, this experiment demonstrates that SFG spectroscopy is an effective method for studying soil bacteria surface groups. Future work using this technique will explore other surface groups on different bacteria, as well as the interaction between bacterial surfaces and actinide metals.

Neutron Activation Analysis. FRANK GARCIA (California State University Fresno, Fresno, CA 93740) FRANK ASARO (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

A hypothesis had been previously developed which suggested that silver abundances detected in ancient pottery indicated that the pottery had been used to store silver money. My research was to improve the sensitivity for silver abundance measurements in pottery using instrumental neutron activation analysis so that the hypothesis could be checked. Samples of pottery excavated in Israel were sent to us by Professor David Adan-Bayewitz from Bar Ilan University in Israel. The samples were ground into powder and about 50 mg. weights were sealed in aluminum capsules. These aluminum capsules were then sealed in quartz tubes and sent to the University of Missouri in Columbia, Missouri for irradiation in a nuclear reactor. After irradiation the quartz tubes containing the Al capsules was returned to LBNL and the capsules were measured with the Luis W. Alvarez Iridium Coincidence Spectrometer. The irradiated aluminum capsules containing the pottery samples were inserted into the spectrometer and measured individually. A computer program for acquiring silver data properly from the spectrometer and calculating silver abundances was also developed. For most single's gamma ray measurements the backgrounds were too high to provide reliable information (i.e. the integrated 'peaks' were sometimes only about 0.3% of the background). Coincidence measurements between pairs of gamma rays had helped to reduce the amount of background in previous studies for other elements. But because of specific characteristics associated with the radioactive decay of the irradiated silver, coincidence techniques did not work here for many of the more intense lower-energy radiations. Coincidences

with the high energy gamma rays of 1384 and 1504 KeV, however did work. These gamma rays had energies above those of 2 very intense ^{46}Sc radiations of 889 and 1121 keV. Prior to this research we were not even sure of the reliability of silver measurements using the single's technique. Based on studies of 16 sets of coincidences, we were able to significantly improve both the reliability and the sensitivity of the silver measurements. The project was very successful and silver abundances in pottery can now be measured with a sensitivity of 0.01 ppm, which is not only sufficient to check the starting hypothesis, but may also provide new insights into pottery usage.

Particulate Carbon and Gas/Particle Partitioning of Aromatic Hydrocarbons in Seattle, Part II: Comparison of Winter Polycyclic Aromatic Hydrocarbons and Wood Smoke Tracer Concentrations.

CLINT HOBERG (The University of Arizona, Tucson, AZ 85719) LARA GUNDEL (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). Airborne semi-volatile organic compounds (SVOC's) have become a topic of recent concern. A particular group of SVOC's, polycyclic aromatic hydrocarbons (PAH's), has been given more emphasis because some of these compounds are carcinogenic. Many of these compounds partition readily between the gas and particle phase, which makes it more difficult to characterize these compounds using conventional sampling and analysis methods. Since these compounds are found in wood smoke, the characterization is important for assessing the health effects of wood smoke. In this study ambient air samples taken in Seattle with Lawrence Berkeley National Laboratory's Integrated Organic Gas and Particle Sampler during the winter of 2000-1 were analyzed using high performance liquid chromatography for a specific set of PAH's. Two software tools were developed and validated for HPLC data reduction. Data were then compared to other data collected during the same time frame for comparison. The PAH concentrations were then compared to particulate EC/OC (Elemental Carbon/Organic Carbon) concentrations. PAH's included the wood smoke marker, retene, which was found primarily in the particle phase. Preliminary results suggest that gas phase PAH correlated well with both particulate organic and elemental carbon (soot).

Particulate Carbon and Gas/Particle Partitioning of Aromatic Hydrocarbons in Seattle: The Relationship between Indoor/Outdoor Polycyclic Aromatic Hydrocarbon Concentrations and Sampling Artifacts for Carbonaceous Particles. RACHELLE MAJESKE (Crafton Hills Community College, Yucaipa, CA 92399) LARA A GUNDEL (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

In response to the national push to learn more about air pollution and its health effects, the EPA funded five particulate matter (PM) research centers in 1999, one of which is the Northwest Research Center for Particulate Matter and Health. The Beacon Hill (BH) area of Seattle, WA, has an air quality monitoring station that makes the area a prime location for collecting samples of PM. Fine particles come from vehicles, as well as seasonal wood burning and other sources. Air samples were collected at Beacon Hill as well as indoors and outdoors at private residences using Lawrence Berkeley National Laboratory's (LBNL) Integrated Organic Gas and Particle Sampler (IOGAPS). These samples were then analyzed for gas and particulate polycyclic aromatic hydrocarbons that are known carcinogens. Our objective was to find correlation between outdoor air pollution as measured at a stationary monitoring site (BH) and actual indoor concentrations to which people are exposed.

The Effect of CH_4 and O_2 Concentrations on CH_4 Oxidation in Wet Tropical Soil. CHARLOTTE CARLSON (Middlebury College, Middlebury, VT 05753) MARK CONRAD (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Microbial oxidation of atmospheric methane (CH_4) in aerobic soils is an important secondary sink for atmospheric CH_4 , accounting for 3-15% of the net atmospheric budget (Born et al, 1990). Methanotrophic (methane-oxidizing) bacteria strongly favor the lighter carbon isotope ^{12}C to the heavier ^{13}C isotope due to the kinetic advantages of ^{12}C . As a result, net CH_4 efflux from soil has a higher concentration of ^{13}C . To determine how different rates of CH_4 oxidation affect isotope fractionation, soil incubations were set up for two treatments, varying CH_4 concentrations in one set (100 ppmv CH_4 , 500 ppmv CH_4 , 1000 ppmv CH_4 , and 5000 ppmv CH_4), then O_2 concentrations in the next set (3% O_2 , 5% O_2 , 10% O_2 , and 21% O_2). Soil samples were taken from a montane rain forest in the Luquillo Long-Term Ecological Research site in northeastern Puerto Rico. Results showed that the rate of CH_4 oxidation varied with different initial CH_4 concentrations, yet did not show any significant change with different initial O_2 concentrations. Regression analysis revealed a negative correlation between the isotope fractionation factor and the rate of CH_4 oxidation for the higher CH_4 treatments (>100 ppmv; $P < 0.001$, $R^2 = 0.86$). Results indicate that isotope fractionation is dependent on the

rate of CH₄ oxidation. The presence of both type I and type II methanotrophs could account for the lack of variation in the rate of CH₄ oxidation under different O₂ concentrations.

Using Terrestrial Radiation to Help with Homeland Security. *EN-RIQUE LOPEZ (California State University, Fresno, Fresno, Ca 93716) THOMAS KNIGHT (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

Natural radiation is all around us; it comes from such places as rocks, soil, and our solar system and varies from place to place. There are types of man made radiation that can be harmful in relatively large doses. This summer, we at the Intensive Research Institute studied natural terrestrial radiation and how air filters can play an enormous role in detecting unwanted radiation. Engine automobile air filters has been one way of studying our environment. Analyzing engine air filters has proven to be a great early-detection method for radioactivity in our environment. Engine air filters capture charged particles in our environment. Also air filters capture microorganisms such as bacteria's and chemicals. This is another great advantage for analyzing air filters. Studying air filters will help develop a standard for individual areas. After developing this control any deviation from this standard can lead to a red flag. Once a red flag has been reached steps can be taken to investigate and remedy the situation.

Analytical Characterization of Heteropoly Acid Containing Proton Exchange Membranes. *JAMES O'DEA (University of Puget Sound, Tacoma, WA 98416) JOHN TURNER (National Renewable Energy Laboratory, Golden, CO 89401).*

Fuel cells using H₂ derived from renewable energy sources and water produce electricity in an environmentally benign process independent of foreign energy supplies. Proton exchange membrane (PEM) fuel cells have the potential to meet the energy needs of a hydrogen-fueled society. DuPont's Nafion™ is the membrane used most commonly in PEM fuel cells; however, above 80°C, Nafion™ loses water and fuel cell performance decreases. We investigated the thermal stability and ion exchange capacity (IEC) of heteropoly acid containing fuel cell membranes and their components. Heteropoly acids (HPAs) are a large group of inorganic molecules with thermal stability reported above 5000°C and proton conductivity when fully hydrated reported as double that of Nafion™. One HPA, H₆[As₂W₂₁O₆₉(H₂O)]*x*nH₂O, and two H₂Rb₄[As₂W₂₁O₆₉(H₂O)]*x* 34H₂O and a-K₆[P₂W₁₆O₆₂]*x* 14H₂O, were synthesized and analyzed for their thermal stability. Thermal analysis was performed using differential scanning calorimetry and thermogravimetry. These tests revealed that nearly 1/3 of the water molecules in silicon tungstic acid, the HPA used in our membranes, are retained at 1500°C, implying similar water retention for the PEM, an improvement over Nafion™. Acid-base titrations were used to gather IEC data, which ranged from 0.455 to 2.140 mmol H⁺/g sample for fabricated membranes and 2.421 to 3.469 mmol/g for sol-gel powders. Nafion™ was tested as having an IEC between 0.783 and 0.825 mmol/g compared to the literature value of 0.9 mmol/g. IEC results for the HPA based membranes were inconsistent, indicating that improvement of test procedures is needed. This research can be used as a guide for fabricating membranes with improved fuel cell performance.

CO₂ Based Purification of Single-Walled Carbon Nanotubes. *CARA HORBACEWICZ (Rochester Institute of Technology, Rochester, NY 14623) MIKE HEBEN (National Renewable Energy Laboratory, Golden, CO 89401).*

Many potential applications of single wall carbon nanotubes (SWNTs) require the ability to effectively and efficiently purify a variety of as-produced nanotube materials. During synthesis, catalyst metals, amorphous carbon, nanocrystalline graphite and graphite-encapsulated metals are incorporated into the material. Currently, the purification of SWNTs has been limited by long time requirements, low yields, high metal contents, and tedious procedures. Therefore, better methods are being strongly pursued. One focus is to reduce the metal content by freeing the metal particles from other carbonaceous matter prior to reflux. The graphitic encapsulation of the nano-sized metal particles keeps them from interacting with the acid used during the purification. Our investigation focused on utilizing thermal oxidation of the graphitic shell in a carbon dioxide atmosphere whereby the encapsulated metal should become exposed and therefore easily removed by acid solutions. CO₂ provides a gentle oxidation atmosphere so that non-nanotube carbon is selectively oxidized, while the nanotubes remain stable. A series of different CO₂ burn temperatures and times were investigated to determine the optimum experimental conditions. In addition to the carbon dioxide studies, a parallel investigation into the effect of the time of the nitric acid reflux on these materials was also surveyed. In both studies, after the purification process was completed, thermogravimetric analysis (TGA), transmission electron microscopy (TEM) and

scanning electron microscopy (SEM) were used to analyze the purified material. It was found that CO₂ oxidation prior to the reflux of the SWNT as-produced materials, improved the purification procedure by reducing the metal catalyst content nearly 50%. In addition, preliminary data indicates that a 10-hour reflux gives the best result of the reflux times we analyzed for samples pre-treated in CO₂, as compared to 16 hours for samples not burned in CO₂.

Comparing Thermal Stability and Molecular Decomposition of Imidazolium Hexafluorophosphate Salts. *BRAD BRENNAN (Drake University, Des Moines, IA 50311) LUC MOENS (National Renewable Energy Laboratory, Golden, CO 89401).*

Energy storage is a critical factor in the advancement of solar technologies that produce electricity by using sunlight as the direct energy source. The goal of the Advanced Storage Project under the US-DOE Concentrating Solar Power Program is to identify and develop thermal storage options with improved economics or operational characteristics for solar parabolic trough energy systems. Ionic liquids are currently being studied as a new and promising class of low-temperature molten salts that may satisfy the operational requirements of high thermal stability combined with a melting point that is sufficiently low such that freezing of the salt is avoided during cold nights. The thermal stability of an imidazolium salt containing bulky tert.-butyl substituents has been found to undergo thermal decomposition at a much lower temperature compared to a salt with an aromatic substituent. Much better thermal stabilities were observed in a salt containing a linear alkyl side chain. The molecular thermal decomposition pathways were determined based on data obtained through Thermogravimetric Analysis and Molecular Beam Mass Spectrometry.

Design and Testing of a Combinatorial Electrochemical Device for Corrosion Studies. *ERIK GARNETT (University of Illinois, Champaign-Urbana, IL 61820) DAVID GINLEY (National Renewable Energy Laboratory, Golden, CO 89401).*

Corrosion is a major problem facing society today. Great progress has been made in corrosion resistant alloys and binary system coatings, but these materials still can breakdown in harsh environments over long periods of time. Ternary system coatings, such as titanium chromium nitride, may provide a solution, but the many compositional combinations make traditional electrochemical methods cumbersome for extensive testing. To address this problem, we designed and tested a combinatorial electrochemical cell to study the corrosion properties of sputter deposited mixed metal nitride thin films. Completely independent polarization and open circuit potential tests were performed in all 11 cells simultaneously, after scribing the thin films to electrically separate each cell. The polarization curves correlated well with visual corrosion observations, but open circuit potential experiments were problematic due to voltage differences between cells. Contributions to these voltage inconsistencies were systematically identified and include: poor solder joints, thermocouple effects, solder joint wetting, and cell contamination. Although the voltage differences have been reduced, they still are significant (about 250 mV or less). In future work, when the voltage problems are all resolved, the cell will be capable of simultaneously and accurately testing 11 different coating compositions using both linear polarization curves and open circuit potential measurements for each 2x2 thin film substrate. Since there is very little sample preparation, this approach increases the experimental testing efficiency by a factor of about 20.

Polymer Based Photovoltaics. *SAMUEL WILSON (University of California San Diego, La Jolla, CA 92122) SEAN SHAHEEN (National Renewable Energy Laboratory, Golden, CO 89401).*

In this work we investigated the adsorption of two different kinds of acceptor molecules on nanostructured TiO₂ and SnO₂. The effectiveness of the adsorption process was probed with a quartz crystal monitor and UV-Vis spectrophotometry. The structured oxide TiO₂ exhibited a higher binding constant, for PoCPI in CH₃CN than did SnO₂ by UV-Vis absorbance spectroscopy. Structured oxides were optimized to have increased surface areas, by increased layer thickness or a more porous structure so as to achieve a higher optical density by UV-Vis spectroscopy. Increasing the surface area of the structured oxide was successfully accomplished by increasing the viscosity of the metal oxide suspension before spin coating. Sonication using an ultrasonic probe also was successful in breaking but the metal oxide particles, allowing them to be cast into uniform thin films.

Pyrolysis of Biomass. *EMILY REITH (University of Colorado, Boulder, CO 80309) MARK NIMLOS (National Renewable Energy Laboratory, Golden, CO 89401).*

This preliminary research explores the products formed during the pyrolysis of biomass in order to better understand the conditions and

materials most valuable for the production of fuels and chemicals. Pyrolysis is the process of heating materials to high temperatures the absence of air. This investigation had two main parts. First, raw materials such as cellulose and protein were pyrolyzed in an oven for 5-15 minutes at temperatures ranging from 170°C to 550°C. The products formed were detected using a molecular beam mass spectrometer. These experiments covered a wide range of starting materials which included the amino acids, proline, asparagine, aspartic acid, and tryptophan all tested with glucose, glyceraldehyde, and a matrix of glucose, pectin, and cellulose. The samples were subjected to different temperatures and combinations of temperatures. It was found that the amount of char remaining depended on the final pyrolysis temperature, and not on the sequence of temperatures it underwent during the experiment. The second part of this investigation involved using a model compound for cellulose, diethoxymethane. This compound was pyrolyzed using a Chen nozzle and the products were collected on a cold salt window for analysis using an infrared (IR) spectrometer. This technique is known as matrix isolation IR spectroscopy and allows for the formation and preservation of products, including radicals. These experiments were performed at temperatures between 750°C and 1100°C in order to eventually determine the rate constant (k) for the formation of the products with a focus on ethanol. This technique was also useful in identifying the products formed, including ethanol, ethylene, and formaldehyde.

Solid Infrared Spectral Analysis of Model Pyrolyzed Biomass Samples Emphasizing Maillard Chemistry. KARL ANDREASEN (Colorado State University, Fort Collins, Co 80523) MARK NIMLOS (National Renewable Energy Laboratory, Golden, CO 89401). Due to projected declines in petroleum production in coming years, scientists are looking for technologies to replace/supplement petroleum as a fuel and energy source. Using a biomass gasification and fermentation platform, ethanol can be produced from biomass for energy consumption. To understand pyrolysis and therefore maximize efficiency and minimize wastes we used infrared spectroscopy to investigate the Maillard chemistry of pyrolyzed biomass samples. Model biomass samples were created using single amino acids in combination with a carbohydrate(s). These model samples were pyrolyzed at graduated temperatures and then ground into a KBr matrix. Using a Fourier Transform Infrared Spectrometer (FTIR) and a diffuse reflectance apparatus, spectra were taken from 650 to 4000 wavenumbers. In all four hundred twenty four spectra were taken. These IR spectra were then analyzed using principal component analysis. As the temperature rose during pyrolysis (typically between 170° and 350° Celsius) it was observed that the alcohol peaks disappeared. Simultaneously, new peaks in the 1700 and 900-675 wavenumber region were found. The triplicate peaks in the 900-675 range are from carbon hydrogen bonds out of plane bending. This indicates the aromatizing of the biomass during pyrolysis. The peak observed at 1700 wavenumbers indicates the formation of a carbonyl, however more investigation will be needed to determine exactly what kind. Proline was observed to catalyze both the disappearance of the alcohol peak and the formation of the aromatic C-H and carbonyl peaks, making these changes come about at lower temperatures. Further work will trace nitrogen through these chemical changes during pyrolysis so that it may be sequestered in the solid phase of biomass during gasification.

Synthesis of Multiple Bolaform Derivatives to be Used in the Construction of Nanostructures. JOSEPH BULLOCK (University of Kentucky, Lexington, KY 40504) JOSEPH BOZELL (National Renewable Energy Laboratory, Golden, CO 89401). Nanotechnology may yield incredible scientific advances in the near future. It promises to utilize the properties found only in microscopic environments to be used in our macroscopic world. The key to unlocking nanotechnology is the control of molecular arrangement, otherwise known as self-assembly. Unfortunately our knowledge of self-assembly is limited by our lack of understanding of how molecules of the same type interact with one another. To further our understanding of self-assembly, a number of different molecules were synthesized. These molecules have the characteristics of a biomimetic class of molecules known as bolaforms. They have highly polarized end groups connected by a nonpolar carbon chain. These molecules are known to self-assemble under the proper conditions to form a variety of structures. Bolaform 1 (bis-1,12-(4,6-di-O-acetyl-2,3-dideoxy-a-D-erythro-hex-2-enopyranosyloxy)-dodecan e) was shown to form fibers that were analyzed with tunneling electron microscopy (TEM). These structures were relatively large with a high aspect ratio. They were all approximately uniform in size. It is believed that these structures are held together through hydrogen-bonding, although the exact mechanism through which these structures form is not yet understood. It is hoped that examining the

self-assembly of other bolaform derivatives will eventually yield understanding of the process of self-assembly.

Adsorption and Reaction of Methanol on Reduced and Oxidized Ceria Thin Films. MATTHEW ROBBINS (The University of Texas at Austin, Austin, TX 78712) DAVID R. MULLINS (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

In order to explore the basic surface chemistry of a commercial catalyst support material, the thermally activated reactions of methanol on highly oriented cerium oxide thin films were studied. Thin films were evaluated using X-ray photoelectron spectroscopy (XPS) to quantify the average cerium oxidation state and Auger electron spectroscopy (AES) to confirm thickness. Temperature programmed desorption (TPD) provided information on surface reaction products and surface intermediates. Methanol is shown to dissociatively adsorb forming methoxy and surface hydroxyl groups. Further surface reactivity is discussed as a function of the average cerium oxidation state and the corresponding existence of surface oxygen vacancies. On the fully oxidized surface two reaction paths compete at 200K leading to hydrogen reuptake and methanol desorption and the desorption of water and formaldehyde, reducing the ceria substrate. Consistent with the role of ceria as an oxygen storage material, this low temperature reaction pathway leading to surface reduction was favored on highly oxidized surfaces and greatly inhibited on the more reduced surfaces. Methoxy is stabilized on reduced surfaces, and, as the degree of reduction increases, additional reaction pathways become accessible. Any remaining methoxy decomposes at 600K, leaving the surface as dihydrogen, carbon monoxide and small quantities of formaldehyde. The high temperature pathway was greatly enhanced for highly reduced surfaces. In this study the role of methanol as a low temperature reductant is explored and the reactivity of cerium oxide is correlated to the presence of Ce₃₊ cations.

Detection of Perchlorate Anion on Silver Colloids Using Near-Infrared Surface Enhanced Raman Scattering. JACQUELINE TIO (Massachusetts Institute of Technology, Cambridge, MA 02139) BAOHUA GU (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Perchlorate anion, currently under proposal to be federally regulated, inhibits thyroid function and causes metabolic and developmental health problems that can ultimately lead to the formation of tumors. Recent risk assessment by the Environmental Protection Agency (EPA) states that the maximum daily intake value of perchlorate should be 30 ig/kg a day, or equivalent to a maximum contaminant level (MCL) of 1 part per billion (ppb) or less in drinking water. The present designated analytical method for detecting perchlorate in water uses ion chromatography; however, this method's lowest detection limit is ~1 ppb and involves lengthy analytical time in the laboratory. Surface Enhanced Raman Scattering (SERS) provides an alternative way to detect perchlorate ions at extremely low concentrations. Through the use of near-infrared laser excitation of adsorbed perchlorate anions on silver colloids, Raman signal intensity can be enhanced by factors ranging from 102 to 1014. In this study, the characteristic Raman shifts and peaks of perchlorate were observed and enhanced by the presence of silver crystal clusters and NaCl. Experimental results have yielded a minimum perchlorate anion detection limit of ~50 ppb, indicating that the use of silver colloids and the addition of NaCl may provide both a chemical and electromagnetic enhancement of the Raman signals for perchlorate due to surface plasmon resonances, sharp crystalline shapes, and modulated charge transfer by chloride anions. Furthermore, the non-linear decrease in probability of locating the presence of perchlorate anions at increasingly diluted concentrations suggests that SERS occurs at specific 'hot' sites non-uniformly distributed throughout a sample. The probability of a perchlorate anion attaching to these 'hot' sites of indeterminate size and, thus, yielding a significant Raman signal fluctuates according to perchlorate concentration and the number of 'hot' sites available. Nevertheless, results indicate, for the first time, that detecting perchlorate anions down to ~50 ppb is feasible through the application of SERS on silver colloids. Further exploration and research may prove to be fruitful in the use of SERS to locate and to detect the presence of perchlorate anions at even lower concentrations.

Dynamic Testing of Pt Electrodes: Hydrogen Formation at the Electrode/Vitreous Humor Interface. MATTHEW WHITFIELD (Vanderbilt, Nashville, TN 37235) ELI GREENBAUM (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Macular degeneration and retinitis pigmentosa are two of leading causes of blindness. In these diseases, photoreceptor cell function is impaired but the rest of the visual pathway remains viable. Therefore, theoretically, if bipolar and ganglion cells could be stimulated directly, some sight could be restored. A possible solution is to have an "artificial retina" consisting of platinum electrodes arrayed on a chip about the size of the fovea, directly implanted onto the retina. A small digital

camera would transmit images to the chip, pulsing the electrodes and stimulating the retinal cells. There is a possibility of producing harmful byproducts in this process. Water can be electrolyzed producing H_2 and O_2 gas, H_2O_2 can form, and Cl^- from $NaCl$ in the eye can react with oxidized Pt from the electrode creating $PtCl_4$ or $PtCl_6$. In this project, H_2 is used as an indicator of all these byproducts and its production is monitored. The more electrodes on the chip, the better the "resolution" and the clearer the images could become. Smaller and smaller wires would be required to fit more and more electrodes on the same size chip. But, for a given current, the smaller the wire the higher the charge density and the more likely the electrolysis of water becomes. The purpose of the project is to determine, for a given size of wire, the maximum pulse times and optimal pulse forms that can be applied to the electrodes without oxidizing Pt or producing H_2 . Electrodes to be tested are immersed in Ames medium which closely resembles vitreous humor and pulsed with currents. This is done in a closed system and a stream of zero air carries all H_2 produced to a tin oxide H_2 sensor. When testing an electrode, a pulse known to produce H_2 is applied, followed by incrementally decreasing pulses until no H_2 is observed. Biphasic pulses produced less H_2 than negative, monophasic pulses. Biphasic pulses with no or 1 msec intraphase delays are comparable and marginally better than biphasic pulses with 5 msec delays. With a 1.05 mm diameter electrode, charge densities have to be less than 1 mC/cm² to prevent H_2 production. With a 75 mm wire, preliminary results show that H_2 is not produced at a charge density of less than 12 mC/cm². It has yet to be determined if the electrode erodes at this charge level but, at higher levels, significant degradation is present. The results will be passed on to electrode manufacturers who will use them to design safe products.

Effect of Substituents on the Competition Between Decarboxylation of Aromatic Carboxylic Acids and Anhydride Formation. KEN-NETH KEARNS (Saginaw Valley State University, University Center, MI 48710) PHILLIP BRITT (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

In the pyrolysis and liquefaction of low rank coals, oxygen functional groups are thought to be responsible for cross-linking reactions that form more refractory products. One potential route to these cross-links is from the formation of anhydrides from the condensation of aromatic carboxylic acids and their decomposition by an induced free radical decay mechanism, which leads to the formation of aryl radicals. These aryl radicals can then add to other aromatic rings to form cross-links. In addition to anhydride formation, aromatic carboxylic acids also undergo decarboxylation via an electrophilic pathway to produce an aromatic hydrocarbon. To determine the effect of substituents on the formation of anhydrides (or its decomposition products) versus decarboxylation, the pyrolysis of various substituted benzoic acids was investigated in vacuum-sealed Pyrex tubes at 400°C for various times. Electron-donating substituents, which accelerate the decarboxylation reaction and potentially inhibiting anhydride formation, was investigated since the aromatic rings in low-rank coals contain electron donating moieties, such as alkyl, methoxy, and hydroxy groups. Since the anhydride may be unstable under the reactions conditions, the pyrolyses were conducted in a seven to ten-fold excess of naphthalene, which traps the radical decomposition products from the anhydride. The pyrolysis products were identified using GC-MS and quantified using GC with a FID with the primary focus on the formation of substituted benzene, anhydride, and cross-linked products. Studies using benzoic acid, p-methylbenzoic acid, m-methoxybenzoic acid, and p-methoxybenzoic acid have shown that the substituents do have an effect on the rates of decarboxylation and anhydride formation. Electron donating groups such as methyl and methoxy groups in the para position do not completely inhibit anhydride formation as initially predicted. The study does, however, indicate that anhydride formation may be a pathway for cross-linking in low-rank coals.

Evaluation of Factors Affecting Cesium Extraction Performance by Calix[4]arene Derivatives. JENNIFER RUMPPE (Beloit College, Beloit, WI 53511) LAETITIA H. DELMAU (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Novel aza-crown derivatives of dioctyloxy-calix[4]arene crown-6 were examined for their cesium extraction performance at different pH levels. These studies are of interest in addressing high-level waste tank remediation and the removal of ¹³⁷Cs, a major contributor to heat and radiation generation. Preliminary studies were done to assess the performance of these calixarene compounds under varying conditions. Results showed an increase of cesium extraction with pH as well as expected trends in diluent effects and anion selectivity. Poor extraction performance of some derivatives raised questions regarding the possibility of intramolecular hydrogen-bonding. A newly synthesized methyl-

ated derivative was used to address these questions. All compounds were assessed for their extraction performance as related to pH. Additional experiments were conducted to determine pH changes caused by extraction at varying levels of acidity and basicity. Results indicate an increase in cesium extraction with pH, as shown in preliminary studies. Mono-aza derivatives were shown to exhibit better cesium extraction performance than their di-aza counterparts. The methylated derivative showed poorer extraction performance than the non-methylated derivative, indicating that completely removing the possibility of intramolecular hydrogen-bonding has negative effects on extraction performance. One possible explanation is that the hydrogen-bonding facilitates anion co-extraction, which would lead to better overall extraction. Mono-aza derivatives were shown to cause unexpected changes in pH. This could possibly be attributed to protonation of the calix crown.

Immobilization and Image Processing of Biomolecules and Nanostructures on Epitaxially Grown Gold Film. ANNA KISIELENTE (Wilbur Wright Community College, Chicago, IL 60632) IDA LEE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Photosystem I (PSI) and Bacteriorhodopsin are photosynthetic proteins naturally embedded in the membranes of the organelles responsible for organism to photosynthesize. PSI can be isolated from spinach and immobilized orientated onto a gold surface. Under a controlled temperature in a high vacuum chamber, ultra pure gold was epitaxially grown as a single crystal film on mica. Individual pieces of gold were submerged into a vial containing 2-Mercaptoethanol. 2-Mercaptoethanol was used to modify the surface of the gold creating a Self Assembling Monolayer (SAM). The sulfhydryl group of the 2-Mercaptoethanol specifically binds to the gold, while the hydroxyl group binds to PSI. Subsequently, all gold samples were incubated in PSI solution in ten second increments from ten to sixty seconds to determine coverage density of PSI on gold. Samples were cleaned, dried and mounted onto stainless steel disks prior to imaging by tapping-mode on the Atomic Force Microscope (AFM). Image processing adjustments such as contrast enhancement, color table changes, edge locator, zoom and removal of scan lines were performed on all images. These techniques were used to rebuild the visibility of the PSI and Bacteriorhodopsin nanostructures and to enhance the image content. Following the appropriate image processing, image files were transferred to NIH Image software for particle counts. Particle count data has been retrieved for all samples. The data shows a significant rise of PSI particles between the ten and thirty second increments. The thirty second sample had a density of 44.62 particles/area. The forty second sample had a density of 46.30 particles/area. Results conclude that even though the area between samples differed, PSI particles on the surface of the gold between the thirty and forty second samples had reached saturation. After the forty second sample, PSI particles began to aggregate in groups, decreasing the number of particles per count, creating difficulty in obtaining accurate particle counts. There also was a difference in quality between the forty and fifty second samples. Particle counts were easy to obtain and PSI particles maintained a distance from one another in the thirty second sample. In the fifty second sample, PSI particles aggregated in groups, making it difficult to obtain an accurate particle count. Particle counts and size distribution analysis between ten and forty second samples showed the best detail, accuracy, and content.

Luminescence of Cu²⁺ and Mn²⁺ Doped. CHRISTOPHER TABOR (Centre College, Danville, KY 40422) T. GREG SCHAAFF (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Nanocrystals of ZnS were prepared by adding Na₂S to a solution of metal ions and glutathione, a naturally occurring peptide chelator. The glutathione acted as a capping ligand to arrest the growth of the ZnS crystals at a size of a few nanometers, and produced nanocrystals that are highly soluble in an aqueous solution. Excitation of ZnS:glutathione nanocrystals at 300 nm induces a broad emission peak centered at 406 nm (violet). Doping the crystals with intentional defects such as Cu₂₊ and Mn₂₊ shifts this emission wavelength to 545 nm (green) and 575 nm (green-yellow), respectively. Powder X-ray diffraction is consistent with native ZnS (sphalerite) structure and does not appear to be altered substantially by the inclusion of Cu₂₊ and Mn₂₊ when the percent doping was relatively low (< 1%). Solutions prepared with higher percent doping resulted in unstable nanocrystals that decompose into small metal complexes or aggregated in large macrocrystals. The effects of variables such as percent doping, concentration of crystals, shelf life, and the presence of O₂ on the luminescence intensity and emission wavelength were studied. Emission wavelengths are consistent with known transitions either from crystal defects in the ZnS core (eg. S₂ vacancies) or interstitial metal ion centers (Cu₂₊ and Mn₂₊). Quantum-size effects are apparent in these nanocrystals manifesting as an increase in the band gap, roughly 0.36 eV higher than bulk ZnS. Other metal ions

were briefly looked at as dopants, such as Co_{2+} and Ni_{2+} , but were not effectively incorporated into the ZnS core. The changes to ZnS electronic structure due to quantum confinement and doping by Cu_{2+} and Mn_{2+} will be discussed for these unique, highly soluble nanocrystals. These changes prevalent in ZnS, a direct band gap semiconductor, may be applicable to other semiconductor nanocrystals (e.g. CdS, CdSe) with direct application to biomedical imaging and nonlinear optics.

Medical Bandages Web Site Project: Research in Economics, Marketing, and Web Design. KATHARINE BAYLOR (*University of Virginia, Charlottesville, VA 22904*) TANYA KURITZ (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

After the fall of the Soviet Union in 1991, reduced defense requirements and a crippled economy forced Russia to downsize its enormous nuclear weapons complex. This consolidation left thousands of scientists with extensive nuclear knowledge and access to nuclear materials unemployed. The U.S. is now faced with a serious threat to its national security as these unemployed workers become tempted to sell their nuclear know-how to the highest bidder, including non-nuclear nations and terrorist organizations. Out of fear of this 'brain drain,' the U.S. has enacted several nonproliferation programs to help Russia safely downsize its nuclear complex. One program in particular, the Nuclear Cities Initiative, is interested in finding alternative, peaceful employment for the released workers. One of NCI's projects involves working with a former plutonium-producing facility in the Russian city of Zheleznogorsk, the Mining and Chemical Combine, which has developed a line of medical bandages. Because few MCC personnel have been trained in advertising and marketing, they are not selling any of their bandages despite a desire for them in the Russian market. NCI is helping MCC build an appropriate manufacturing and marketing infrastructure. By using the Internet as a research tool, establishing contact with MCC officials, reading company documents and information from NGOs, and interacting with a knowledgeable and experienced mentor, the author has gained an increased understanding of the Russian economy and markets, and consumer trends of the Russian people. Using this knowledge, and with assistance from a computer programmer and a Russian translator, the author designed and wrote a bilingual web site that is clear, informative, and professional-looking. The site was designed to be accessible to the Russian people, the Russian Ministry of Health, and non-profit organizations such as the Red Cross. This diverse audience was targeted in order to bring increased attention to the bandages and find interested consumers. In the long run, the site will help sustain the medical bandages production facility, enabling the former nuclear workers at MCC to continue working in a non-weapons environment. In the wake of September 11th, amidst increased fear that terrorists might acquire the knowledge and materials to construct a nuclear weapon, it is necessary for the U.S. to continue to provide employment opportunities such as this one for the displaced Russian scientists.

Room Temperature Ionic Liquids Separating Organics From Produced Water. WHITNEY RIDENOUR (*Roane State Community College, Harriman, TN 37748*) JOANNA MCFARLANE (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Room Temperature Ionic Liquids (RTILs) are salts that are liquid at room temperature with low-vapor pressures, suggesting they are green solvents that will not destroy or deplete the environment. Changing the anion or cation can vary their viscosities and chemical properties to suit a specific purpose. The goal of this research is to investigate a clean, effective, environmentally-friendly way to purify produced water. The experiment conducted was to test the effectiveness of RTILs in pulling organics out of the aqueous phase under different tested conditions. The aqueous phases were then analyzed on a High Performance Liquid Chromatograph or extracted with methylene chloride and measured with a Gas Chromatograph and then compared to controls. Only small amounts of organics were used (1g/L or in some cases 100 g/L solutions). The results thus far are good with distribution coefficients for some organics over 500. Hexanoic acid is pH sensitive, as the protonated form is better pulled out of the produced water by the test RTIL (Bmim Tf₂N) than the non-protonated form. 1-Nonanol is also pH sensitive but the non-protonated form is being pulled out by the RTIL (Bmim PF₆). This demonstrates that the RTIL can be recycled because the RTIL should be able to extract the organic out of produced water and then a high or low pH rinse solution can be used to de-protonate or protonate and pull the organic out of the RTIL. The RTIL can then be reused for another extraction, and the organic can be disposed of properly.

Separation of Free Acid Porphyrins Using Reversed-Phase High Performance Liquid Chromatography. MARILYN DE APODACA (*Florida International University, Miami, FL 33199*) GARY J. VAN BERKEL (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Porphyrins are a class of naturally occurring compounds present in all living organisms. Porphyrins all share a common structure that consists of tetrapyrrolic subunits linked by methylene bridges; it is an aromatic system that contains 22 pi electrons. Distinct substituents transform the porphyrins leading to a variety of structurally analogous compounds; for example, the six free acid (or non-esterified) porphyrins- 8, 7, 6, 5, 4, and 2 carboxylporphyrins -differ by the number of carboxylic groups found throughout the ring structure. The separation of the six macrocyclic porphyrin acids (10 nmol/mL) was accomplished using Reversed-Phase High-Performance Liquid Chromatography (RP-HPLC) and detected using a UV/VIS diode array detector with the optimal wavelength $\lambda = 400$ nm. A gradient elution method was developed to resolve the six macrocyclic porphyrin acids. The three different reverse phase columns used - Zorbax ODS, BetaBasic18, and Jupiter - all employed an octadecyl (C_{18}) bonded phase; however, the pore sizes varied from 70 to 300 Å. The separations of the macrocyclic non-esterified porphyrins were strongly dependent upon the pore sizes of the columns. The Zorbax ODS and BetaBasic18 columns did not provide an adequate separation for the six porphyrin acids. The Jupiter column, which was the shortest of the three but also which had the largest pore size, permitted complete resolution for the six components with a run time under 11 minutes. A gradient elution method was developed for the Jupiter column to resolve the six macrocyclic porphyrin acids. The most effective gradient composed of an initial solvent of 78/22 0.1% formic acid/acetonitrile (hold for 8 minutes), changing to 100% acetonitrile in 2 minutes, then re-equilibrated back to the original solvent composition after 14 minutes. The flow rate for the Jupiter column was 0.5 mL/min.

Shedding Light on Glycolysis. ADAM FARLEY (*Murray State University, Murray, KY 42071*) MITCH DOKTYCZ (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Biological processes are characterized by complex methods of regulation that allow a cell to adjust to its environment. Cell metabolism is one of the most studied of these pathways and operates through a vast network of feedback regulation. Glycolysis was the first major enzyme system in metabolism to be described in detail and has revealed several methods of control. The committed step of glycolysis is the conversion of fructose-6-phosphate to fructose-1,6-bisphosphate with the enzyme phosphofructokinase (PFK) and ATP. Prior investigations have shown that the reaction oscillates between limiting values of reactant and product under the proper conditions of feedback activation and inhibition. As the reaction oscillates, the levels of substrates fluctuate periodically, and each can be monitored to determine how the reaction is proceeding. The traditional method is to couple one of the species to a reaction that converts NADH to NAD and monitoring the subsequent change in absorbance at 340 nm, but this involves the addition of a complicated enzyme system. A simpler approach would be a direct measurement of ATP concentration. Using the chemiluminescent reaction of luciferase to convert ATP to ADP with luciferin is a novel method to monitor the progress of the PFK reaction. This reaction yields a quantitative reflection of ATP levels that is extremely sensitive (picomolar range). This system has the benefits of using fewer coupling enzymes and allows signal detection to be simplified creating options for different reaction vessels. Experiments have shown that the two reactions can proceed in the presence of all the necessary enzymes and reactants, and the ATP signal is still a quantitative function of concentration in the presence of PFK and substrates. The oscillating reaction system requires the use of a flow cell that can isolate the enzymes in a reaction chamber, and recent attempts have been successful in creating an appropriate cell with available materials. The next step is to determine the optimum operation conditions to produce oscillatory behavior using the traditional coupled enzyme system and then using these conditions to produce an oscillating signal with the luciferase assay. The ultimate goal of the research is to be able to use this reaction system in nanoscale cellular mimics to produce a signal that can vary as the cell mimic is exposed to different conditions of feedback effectors.

Single Molecules on Solid Surfaces and Biomolecular Electronics. TAMMY CHANG (*University of Tennessee, Knoxville, TN 37996*) IDA LEE (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

One of the essential components of biomolecular electronics is bacteriorhodopsin, a purple pigmented protein found in the outer membrane of a bacterium that converts light energy into chemical energy in the synthesis of ATP. Another important component is Photosystem I (PSI) reaction centers which are pigment proteins isolated and purified from green plants. The surface charge density of a bacteriorhodopsin membrane can be derived from its potential energy in nanometer resolution. Surface charge density is proportionally related to its surface potential energy measured by scanning surface potential microscopy (SSPM). By applying an equation that links surface charge density to potential

energy, the average surface charge density of bacteriorhodopsin under different lighting can be calculated and represented by three dimensional surface plots generated in MathCad. A procedure other than X-ray to measure the PSI size distribution was developed. It involves growing an atomically flat gold surface on mica substrate in a vacuum chamber over several weeks. The pressure inside the vacuum chamber was measured by an ion gauge and maintained at or near 10^{-6} torr. Round pieces of gold films were cut out. Self-assembled layers of PSI concentration are then immobilized on the gold film by 2-mercaptoethanol at various incubation times ranging from 10 seconds to 1 minute, with an increment of 10 seconds. The samples were characterized by the tapping mode of an atomic force microscope (AFM). Samples are sectioned to learn about their surface profiles to help determine the PSI coverage density and size distribution. The images obtained by the AFM were enhanced by Adobe Photoshop Elements to distinguish individual PSI particles and threshold the grayscale image to binary. Particle counts were accomplished by using an image processing and analysis program similar to NIH Image to find the ratio between the area occupied by PSI and the total gold area. The PSI coverage density was found to be increasing at the rate of $7.0 \ln(x) - 0.96$ % per second as incubation time increases, which supports the hypothesis that the longer the gold has been incubated, the higher the chance that it is more densely covered by PSI. By measuring the area of each individual PSI particle at various incubation times, it is concluded that incubation time is not a factor in the result of the size distribution of PSI, since particle sizes at different incubation times are found to be very similar.

Surface Sampling Aspects of Electrospray Mass Spectrometry. JONATHAN LLAVE (Florida International University, Miami, FL 33199) GARY VAN BERKEL (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

It has recently been demonstrated that Thin Layer Chromatography (TLC) can be coupled directly to a mass spectrometer using Electrospray ionization (ESI) (Van Berkel et al., 2002). The purpose of this research is to develop separations to be used in advancing the TLC/ESI-MS system. Using reversed-phased C18 TLC plates by Merck, the separation of the following systems will be discussed: Test Dye Mix III (a combination of fast green FCF, fluorescein, naphthol blue black, and rhodamine B), Goldenseal extract (berberine, palmatine, hydrastine, and hydrastinine), and a Porphyrin Acid Marker kit (8-carboxyl porphyrin, 7-carboxyl porphyrin, 6-carboxyl porphyrin, 5-carboxyl porphyrin, 4-carboxyl porphyrin, and mesoporphyrin IX). All samples were dissolved in methanol, and then 1 μ l aliquots were spotted on the TLC plates. Using conventional TLC equipment, partial separation was obtained for Goldenseal, and full separation was obtained for the other systems; all of these systems are feasible for analysis with TLC/ESI-MS. Visualization of non-visible compounds was done with a 365 nm ultraviolet lamp. This work is only a portion of a larger project dealing with TLC/ESI-MS.

Binding studies of Actinides and Lanthanides Using a Novel Phosphorus-Based Ligand System. CUTHBERT MARTYR (University of the Virgin Islands, Charlotte Amalie, VI 00802) KIA RICHARDS (University of the Virgin Islands, Charlotte-Amalie, VI 00802) GREGG LUMETTA (Pacific Northwest National Laboratory, Richland, WA 99352). Liquid-liquid and liquid-resin separations are important tools used in the treatment of radioactive waste. A new phosphorus ligand based system has recently been developed and was used to investigate the liquid-liquid and liquid-resin extraction of actinide ions under varying acid type, acid concentration, and ligand concentration. The ligand studied was $(\zeta^5\text{-pentamethylcyclopentadienyl})\text{tris}(\text{-diethylphosphito-P})\text{cobalt(III)}$, $\text{Cp}^*\text{Co}[\text{P}(\text{O})(\text{OEt})_2]_3$, which is a derivative of a class of ligand studied extensively by W. Kläui and others. Liquid Scintillation Counting (LSC) and Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) were used to obtain the data used to determine equilibrium distribution constants for the systems studied, yielding information regarding the relative selectivity of these systems. Binding of La^{3+} and the ligand, in the solid state and in solution, was studied using Raman Spectroscopy.

Bulk Binding Studies of Oleic Acid to Cotton. ANDREW MASHCHAK (Columbia Basin College, Pasco, WA 99301) STEVE C. GOHEEN (Pacific Northwest National Laboratory, Richland, WA 99352). Elastase is released in chronic non-healing wounds by neutrophils, a type of white blood cell. Excess elastase in a wound can digest much needed growth factors and tissue, thereby slowing the healing process. Serum albumin has been shown to moderate elastase activity and thus its sequestration is a potential means of chronic wound remediation. One method of sequestering albumin is through binding to oleic acid. In this research, the feasibility of producing a surface capable of inactivating albumin by binding oleic acid to cotton was examined. Bulk studies were carried out by mixing ground cotton with a solution of oleic acid. After allowing time for the oleic acid to bind, the samples were centri-

fuged and the supernate analyzed to determine the amount of oleic acid which remained in solution. The difference between this and the original concentration was compared against a calibration curve to determine the amount of oleic acid bound to the cotton. Several different concentrations of oleic acid were used to determine the maximum amount of binding which could occur. Results indicated that no significant binding of oleic acid to cotton occurred.

Characterization of the ispF Protein in the Nonmevalonate Pathway of *Shewanella oneidensis*. GREGORY MARSING (Brigham Young University, Provo, UT 84606) NANCY G ISERN (Pacific Northwest National Laboratory, Richland, WA 99352).

Isoprenoid biosynthesis is essential in the life of all organisms playing a role in electron transfer, metabolism, photosynthesis, membrane stability, and in cell signaling. In the synthesis of isoprenoids there are two pathways available, the mevalonate pathway and the nonmevalonate pathway. The mevalonate pathway is utilized in mammals and fungi, while bacteria, plant cell plastids, and apicomplexan parasites make use of the nonmevalonate pathway for the synthesis of isoprenoids. Since the nonmevalonate pathway is used by apicomplexan parasites and is not by mammals it presents itself as an ideal target for designer medication. Not all of the intermediate enzymes involved in the nonmevalonate pathway are characterized. We use genetically altered *E. coli* bacteria to produce SO3437, the *ispF* protein from *Shewanella oneidensis*. From the purified protein, crystals are grown for analysis using an X-ray diffractometer. The data from the diffractometer is then used to characterize the protein structure.

Chemimetric Study of Trichloroethylene Oxidation Using the Fenton's Reagent. ERNEST BRADLEY (Tallahassee Community College, Tallahassee, FL 32304) ERIC W. HOPPE (Pacific Northwest National Laboratory, Richland, WA 99352).

The Fenton's reagent produces a hydroxide (OH^-) radical that is capable of degrading chlorinated solvents such as trichloroethylene (TCE). TCE is one of the most common environmental contaminants in the air, soil, and groundwater. It is used in most applications as a degreaser or dry-cleaning solvent due to its relatively high density and also somewhat low volatility. This bench-scale study examined several methods to optimize the use of the Fenton's reagent on TCE in order to eradicate the highly toxic organic contaminant. The mixture of 300 parts-per-million of TCE in water, an aqueous solution of iron (II) sulfate, diluted sulfuric acid, and Hydrogen Peroxide generated both gas and liquid samples to analyze. The analysis of the liquid phase and gas phase samples were performed using an Hewlett-Packard (HP) 7694 Headspace Sampler connected to an HP5890 Series II Gas Chromatograph interfaced to an HP 5972 Mass Spectrometer. Several parameters were varied to achieve the optimal degradation of TCE such as pH levels, pressure, temperature, reaction time, iron concentration, and dosage levels of hydrogen peroxide. Data generated by the chemical oxidation of TCE indicated maximum degradation of the chlorinated solvent when the pH level was maintained between 2.5 and 3.5, the iron concentration (as Fe^{2+}) was at 0.2 weight percent, and a 12% oxidant loading using 30 percent hydrogen peroxide. Results of the mass balance calculations yielded a 96 percent removal of trichloroethylene from a 300ppm concentration of TCE. It was observed in later examination of the data gathered that pH level and iron concentration are the most vital parameters toward successful removal of TCE.

Hydrogen Reduction of Cis-2-buten-1-ol: A Kinetic Model Evaluation of Hydrogenation versus Isomerization. AMY WILLIAMS (Gonzaga University, Spokane, WA 99258) ROBERT DISSELKAMP (Pacific Northwest National Laboratory, Richland, WA 99352).

Ultrasound at 20 kHz was applied to the isothermal (298 ± 2 K) heterogeneous catalytic hydrogenation of cis-2-buten-1-ol and compared to a conventional experiment in which magnetic stirring replaced the sonic probe in facilitating the reaction. Hydrogenation employed hydrogen gas at 6.8 atm and a catalyst pre-reduced by ultrasound. Palladium black, Raney Nickel, and Pt-doped Raney Nickel were all used in separate experiments. This study was undertaken to examine the effect of ultrasound on the competing reaction processes of isomerization to trans-2-buten-1-ol relative to hydrogenation to 1-butanol. Sampling of the reacting solutions at pre-determined time intervals followed by ex-post-facto GC/MS analyses yielded time-dependent product state distribution information. The concentrations of all products and reagent were graphed with respect to time of reaction, and a kinetic model was developed that fit the experimental data with probable mechanistic pathways for the reaction. From the process of kinetic modeling it was found that the original reagent almost exclusively passes through the isomerized trans-2-buten-1-ol intermediate before converting to the hydrogenated 1-butanol form. It was also found that the application of

ultrasound to the reaction increased the ratio of 1-butanol to trans-2-buten-1-ol by approximately 79% over the comparable stirred experiment.

Hyperthermal energy collisions of CF_3^+ ions with modified surfaces: surface-induced dissociation. TALAYEH REZAYAT (*santa monica college, santa monica, ca 90405*) ANIL SHUKLA (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The dissociative scattering of low-energy ions, especially polyatomic ions, from surfaces has become an active area of research in chemistry, physics and material sciences. The interaction between an ion and a surface is more complicated than ion and gaseous neutral collisions and needs to be explored in detail to understand the ion excitation and dissociation phenomena associated with Surface-induced dissociation (SID) of ions, a technique used for the analysis of high mass ions from biological molecules. However, dynamics studies of SID have been performed only for a few simple systems, viz., ethanol, acetone, benzene and carbon disulfide ions. We have therefore undertaken a study of the SID of a small polyatomic ion, CF_3^+ , at several collision energies between 28.8 eV and 159 eV in collision with fluorinated alkyl thiol on gold 111 crystal. These experiment were performed using a custom built tandem mass spectrometer where the energy and intensity distributions of the scattered fragment ions were measured as a function of the fragment mass and scattering angle. In contrast with the previous studies of the SID of ethanol and acetone cations where the inelastically scattered primary ions dominated the collision process (up to ~50 eV maximum energy used in those experiments), we did not observe a measurable abundance of inelastically scattered undissociated CF_3^+ ions up to the lowest energy studied here. We observed all fragment ions, CF_2^+ , CF^+ , F^+ and C^+ at all energies studied with the relative intensity of the highest energy pathway, C^+ , increasing with collision energy. Also, the SID efficiency decreased significantly as the collision energy was increased from 106 eV to 159 eV. The energy distributions of all the fragment ions showed two distinct components, one corresponding to the loss of nearly all of the kinetic energy and scattered over a broad angular range while the other corresponding to smaller kinetic energy losses and scattered closer to the surface parallel. The latter process is due to delayed dissociation of excited ions after they have passed the collision region and the energy analyzer as excited parent ions.

On-Line Analysis of Organic Compounds in Diesel Exhaust Using Proton-Transfer-Reaction Mass Spectrometry. MEGAN WHITE (*Sacramento City College, Sacramento, CA 95822*) TOM JOBSON (*Pacific Northwest National Laboratory, Richland, WA 99352*).

In this study, diesel exhaust (DE) was measured in real time using a proton-transfer-reaction mass spectrometer (PTR-MS) to determine the effect of an after-treatment catalyst on gas phase volatile organic compounds (VOCs). DE after-treatment catalysts are being designed to reduce the pollutants in exhaust, which contains both particulate matter and gas phase constituents. The PTR-MS can make in-situ real time measurements of hydrocarbons in the air, from concentrations in the parts per million by volume (ppmV) down to the low part per trillion by volume (pptV) range. Spectrum scans were performed at varied engine loads from mass range m/z (mass to charge ratio) = 20 to 200. This showed the relative abundance of gas phase VOCs produced as the engine ran between idle mode and 80% of its maximum load. The mass spectrum was complex and appeared to be composed of aromatic species ionized by PTR ($M+1$) through the anticipated proton transfer reactions as well as unexpected alkane fragments, evidenced by a strong $14n+1$ ion pattern showing intense peaks at $m/z = 43, 57, \text{ and } 71$. A number of protonated $M+1$ masses could be identified. These compounds displayed $M+2$ peaks consistent with known ^{13}C isotopic abundance. As the engine load increased, the concentrations of over 90% of the species decreased. An attached smoke meter showed that soot concentrations increased over the same conditions. In addition, the decrease in the concentration of compounds with a larger molecular weight ($m/z > 100$) was greater than the rate that the smaller compounds experienced. This appears to be due to the affinity of VOCs, larger masses in particular, to adhere to soot particles. Further PTR-MS measurements of VOCs on soot confirmed this by producing a mass spectrum comprised of masses predominantly over 100 amu. On-line analysis of diesel exhaust by PTR-MS is a practical tool for quantifying selected organic species in diesel exhaust and should prove useful for developing better diesel exhaust after-treatment system.

Remediation of Trichloroethylene by Modified Fenton's Reagent. LAURA KUNKEL (*Brigham Young University-Idaho, Rexburg, ID 83440*) ERIC HOPPE (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Trichloroethylene (TCE) is a volatile contaminant that was once widely used as a solvent, and as an ingredient in adhesives, paint removers, typewriter correction fluids, and spot removers, and in the manufactur-

ing of organic chemicals and pharmaceuticals. This has resulted in the widespread contamination of soils and groundwater in various locations where TCE was extensively used. Toxic effects of this carcinogenic chemical include symptoms similar to alcohol inebriation, malfunction of the nervous system, liver and lung damage, abnormal heartbeat, and coma. Higher concentrations can have a narcotic effect, and deaths after heavy exposure have been attributed to ventricular fibrillation. TCE is harmful through ingestion, inhalation and absorption through the skin. The degradation of TCE by modified Fenton's Reagent (iron catalyzed hydrogen peroxide) was investigated to test the feasibility of using the method to eliminate TCE from areas with contaminated groundwater and soil. An array of parameters was tested, including: TCE concentrations, iron concentrations, temperature, system pressure and pH levels. The results of each reaction were analyzed using gas chromatography/mass spectroscopy. On average, the percent removal of TCE was 94. The tests showed that a reduced reaction temperature significantly decreased the amount of TCE removed from the system. Tests also indicated that the amount of iron available directly affects both the reaction rate and the amount of TCE removed. All other tests on the pH, pressure, and system mobility showed no significantly different results from the optimum conditions (12% oxidant loading, 1% iron loading, pH 3.0). These results indicate that Fenton's Reagent may be used as effective method for TCE remediation.

Saliva for Use as a Non-Invasive Biomonitoring Matrix. ALYSSA ROSENQUIST (*Roane State Community College, Harriman, TN 37854*) JAMES CAMPBELL (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Blood and urine are biomonitoring matrices that have been used for the detection of drug exposure and environment contaminants. Saliva is easily obtainable and has been suggested for use as a non-invasive biomonitoring matrix[1]. This project intends to develop a reliable method of detecting organophosphate insecticides, Chlorpyrifos (CPF), O,O-diethyl-O-3,5,6-trichloropyridyl phosphorothioate and its major metabolite, 3,5,6-trichloropyridinol (TCP) in the saliva of exposed rats through the use of negative ion chemical ionization mass spectrometry and selected ion monitoring. The procedure involves exposure of male rats to CPF in doses of 1, 10, and 50 ng/kg and collecting blood and saliva samples at 3, 6, and 12 hour post dosing for analysis of TCP and CPF. The following extraction method in preparing each sample for analysis was developed: trichlorophenol was eliminated as a surrogate and replaced with the labeled trichloropyridinol to achieve the highest recovery percentage possible. Preliminary results indicate that the major metabolite TCP can be recovered between 80-90%, with a standard linear range of 1-50 ng/mL, and an estimated limited detection level of 5ng/mL, thus showing that saliva has the potential of being utilized as a non-invasive biomonitoring matrix. If saliva proves to be an accurate biomonitoring matrix, the referenced procedure can then be used for the detection of disease as well as exposure to various toxic organic chemicals. With newly emphasized national security issues, this technique has applications to chemical warfare and threats of bioterrorism. Detection of the agents provides crucial information for saving lives by enabling physicians to diagnose each patient and administer treatment before serious damage occurs throughout the body. This technique provides a readily accessible tool in detection and opens the door for its use as a biomonitoring matrix in future medical research, thus enhancing technology in medical science as a whole.

The In Vivo Quantitation of the Organophosphorus Insecticides Diazinon, Chlorpyrifos, and Their Major Metabolites in Rat Blood Using Gas Chromatography with Nitrogen Phosphorus and Flame Ionization Detectors. ANDREA BUSBY (*Trinity Western University, Langley, BC, V2Y 1Y1*) CHARLES TIMCHALK (*Pacific Northwest National Laboratories, Richland, Washington 99352*).

Chlorpyrifos (CPF)(O,O-diethyl-O-[3,5,6-trichloro-2-pyridyl]-phosphorothioate, CAS 2921-88-2), and diazinon (DZN)(O,O-diethyl-O-2-isopropyl-4-methyl-6-pyrimidyl thiophosphate, CAS 333-41-5) are commonly encountered organophosphorus insecticides whose oxon metabolites (CPF-oxon and DZN-oxon) have the ability to strongly inhibit acetylcholinesterase, an enzyme responsible for the breakdown of acetylcholine at nerve synapses. Chlorpyrifos-oxon and DZN-oxon are highly unstable compounds that degrade via hepatic, blood, and intestinal metabolism to the more stable metabolites, TCP (3,5,6-trichloro-2-pyridinol, CAS not assigned) and IMHP (2-isopropyl-6-methyl-4-pyrimidinol, CAS 2814-20-2), respectively. Studies have been performed to understand and model the chronic and acute toxic effects of CPF and DZN individually but little is known about their combined effects. The purpose of this study was to improve pharmacokinetic/ pharmacodynamic (PK/PD) computational models by quantifying concentrations of CPF and DZN and their metabolites TCP and IMHP in rat blood, following exposure to

the chemicals individually or as a mixture. Male Sprague-Dawley rats were orally dosed with 60 mg/kg of CPF, DZN, or a mixture of these two pesticides. When administered individually DZN and CPF were seen to reach their maximum concentration at ~3 hours post-dosing. When given as a mixture, both DZN and CPF peak blood concentrations were not achieved until ~6 hours post-dosing and the calculated blood AUC for both chemicals exceeded those calculated following the single dose. Blood concentrations of IMHP and TCP correlated with these findings. It is proposed that the higher AUC obtained for both CPF and DZN as a mixture resulted from competition for the same metabolic enzyme systems.

Zinc-67 Solid State Nuclear Magnetic Resonance of Systems of Biological Interest. AMY CARR (Fort Lewis College, Durango, CO 81301) ROBERT W. HECK (Pacific Northwest National Laboratory, Richland, WA 99352).

Zinc is a required trace element for all eukaryotic life. Proteins containing zinc ions constitute over 3% of human gene products. Zinc may play a structural role or be involved in the catalytic functions of these proteins. Specifically we are looking at zinc fingers, a type of DNA binding domain that is primarily involved in gene transcription. The current understanding of zinc finger structure is qualitative. In order to grasp the intricacies of the zinc finger domain function a quantitative understanding of the chemical environment must be attained. The main focus of our group is to develop the technique of solid-state ^{67}Zn nuclear magnetic resonance (NMR). A unique combination of well-established pulsing techniques allows us to collect spectra that have previously been unfeasible with such a nuclide as zinc. Using a specialized ^{67}Zn probe at a temperature of 10 K we are able to determine the chemical environment of the zinc directly. Due to its electronic configuration, there is no other spectroscopic method available to look exclusively at the structural and electronic environment surrounding zinc. In this study the protein BKLF, which has a Cys₂His₂ zinc finger domain was inspected. Additionally a zinc finger analogue was synthesized for analysis. The information we are acquiring serves to elucidate the vital role of zinc in biological systems.

COMPUTER SCIENCE

3D Visualization Toolkit. SHUAIB CHOWDRY (Pace University, NYC, NY 11103) SZE MAN CHAN (Pace University, New York, NY 10038) GREGOR VON LASZEWSKI (Argonne National Laboratory, Argonne, IL 60439). H. WINKLER (Argonne National Laboratory, Argonne, IL 60439).

The Network for Earthquake Engineering Simulation (NEES) is a NSF sponsored nation-wide grid computing project to simulate the structural reactions to earthquakes both physically and numerically [1]. Paul Hubbard in the Department of Mathematics and Computer Science at ANL is conducting a scaled-experiment. Our FaST team project has developed a 3D visualization software prototype to mimic these scaled, laboratory earthquake engineering simulations within a virtual world. The software program allows various users to monitor both the animation of building vibrations and laboratory experiments due to ground shakings in workstations. A reduction of time in research specific details of earthquake engineering can be achieved through grid computing by displaying the 3D model on a workstation using high performance programming language in Java 3D. We can visually recapture the ground motions and the movements of buildings or objects not only in numerical data, but also through 3D demonstrations directly driven by physical sensor data streaming in from a remote site. All these can be performed on a controllable graphical user interface. This software prototype includes three main components: a motion control library, a set of visual representation of an architectural structure in 3D and a graphic user interface to control the visual experiment. The motion control library, which can be applied to the data from the shake table, is responsible for the data representation, data streaming, building client/server environment and representing sensors and vibrations of the building. The architectural structure is consisted of layers of scene features and a set of architectural objects to represent the virtual building and sensors. A set of behavior functions, which allow direct data driven or user interaction, are used to simulate the building motions in time. The viewer, which integrates both data streaming and the visualization, contains the functionality of 3D object manipulation, data import/export and manages the behavior functions. We have explored two types of behavior controls, which can vividly reflect the building vibrations due to shaking. One is to construct all geometrical objects and use the sensor data to drive the object motions. The advantage of this approach is that the sensor data can be applied in real-time exactly like how earthquake has occurred to a building. However, the limited sensor data would require an extensive

extrapolation of the behavior function to reflect all motions. We have assumed that the same floor has the same behavior function to reduce the number of the behavior control. The other behavior control would be to construct a vertices-based structure where each forms a motion frame. By controlling only a few vertices movements, we can easily achieve the motion behavior. The deformation of building can vividly be simulated in this approach. However, the frame forming approach requires buffering a certain number of time frames.

A Comparative Performance Analysis of the Java CoG Kit. MIHAEL HATEGAN-MARANDIUC (Illinois Institute of Technology, Chicago, IL 60616) GREGOR VON LASZEWSKI (Argonne National Laboratory, Argonne, IL 60439).

The benefits offered by the Grid architecture have resulted in the tremendous growth of the Grid-user community. The Globus toolkit has emerged as the most popular Grid implementation used by the Grid community. The Java CoG Kit provides a rich suite of artifacts and client-side constructs to access the backend Globus enabled Grid functionality. This paper is motivated by the need to evaluate the tradeoffs, made by the underlying infrastructure, in choosing either a native Globus client interface or a Java CoG Kit provided interface. This paper does not attempt to prove the superiority of one mechanism over the other, rather it offers decision aiding data to help client developers choose the appropriate service access mechanisms based on their application requirements.

An Investigation of Local Search Strategies for Equational Satisfiability. KEN KEEFE (Southern Illinois University - Carbondale, Carbondale, IL 62901) WILLIAM MCCUNE (Argonne National Laboratory, Argonne, IL 60439).

The search for models of algebra is a very important and demanding aspect of Automated Reasoning. Typically, a model is represented in the form of a matrix or a set of matrices. When a model is found that satisfies all the given theorems of algebra, it is called a solution model. This paper considers algebras that can be represented using a single operation, by way of the Sheffer Stroke. The characteristic of needing only one operation to represent an algebra reduces the problem by requiring a search through all instances of a single matrix. This search is a simple thing to do when the domain size is small. In the case where the domain size is 2, a matrix will have two rows, two columns, and each cell can contain the value 0 or 1. The search space for such a problem is trivial because there are 2^{2^2} or 16 distinct (possibly isomorphic) instances of matrices. When you consider a domain size of 10 however, the search space increases dramatically. With domain size 10, a matrix will have 10 rows, 10 columns, each cell can contain a value from 0 to 9, and $10^{10 \cdot 10}$ or 10^{100} distinct (possibly isomorphic) instances of the matrix. Hypothetically, if it took 1 microsecond to check a single instance of a matrix, then it would take 3.2×10^{86} years to check every one of those 10^{100} matrices. It is clear that a method better than this brute force global search is desirable. Most modern model finding programs like MACE4 use a global search that, instead of merely checking every possible matrix, the programs will use some set of heuristics that will allow the search space to be dramatically smaller and the possibility of reaching a solution more reasonable. Another possible path is local search. This paper discusses local search and several local search strategies that were applied to the problem of equational satisfiability as described above. It is the author's hope that the content of this paper will serve as a road map of strategies and also as a tool of inspiration for future local search strategies.

Analysis of the Waste Management System's Paper Requisition to Develop the Web Requisition Using ASP Programming Language. ANDREW LOBBAN (Richard J. Daley College, Chicago, IL 60607) D. KETO (Argonne National Laboratory, Argonne, IL 60439).

The Project entails the analysis of Waste Managements System's (WMS) paper requisition to generate a web-like requisition that will eliminate the current paper process. The web requisition is developed with Active Server Pages (ASP), HTML, JavaScript and several programming languages like SQL (Structured Query Language). The design of the web requisition (webreq herein) is similar to the current paper requisition in design so that waste generators, and any other users, are familiar with what information they should supply. The student's task was to make the webreq more user-friendly, robust and secure. To accomplish this, additional features were implemented to protect the program's integrity. These features include User Authentication, Saving Users' Information, and Saving Changes. There were also certain important features that had to be put in place: 1) A Role – This feature obtains the user's information, which includes the person's level of access. The role is the user's passport to validate his or her access in the application. The role can either allow or deny the user access to certain data entry fields based on the access related to those fields. A user has

to complete a required Environmental Safety Hazard (ESH) training course before any access is granted for use of the application. 2) Dual Roles – Certain users may have dual roles that grant them access to data entry fields in the application that they may not have access to with a singular role. For example, a user may be a Waste Generator and a Health Physicist technician. Scenario: A waste generator can access all generator specific data entry fields. A health physicist can access only health physics related data entry. An individual with waste generator and health physics roles can access both waste generator specific and health physics specific data entry fields, provided the individual with the dual roles is also the creator of the requisition. Otherwise, the individual may only look at another waste generator's generator-specific input. In this case, only the health physics data entry fields are available for input. The other information is simply informational only.

Cathode Development for Use in Fuel Cells. JEREMY LAWLER (Southern Illinois University, Carbondale, IL 60439) J DAVE CARTER (Argonne National Laboratory, Argonne, IL 60439).

A brief introduction to the procedures used to develop a cathode slurry used in both fuel cells and electrochemical pumps. Reviews components of the slurry, their function, and what procedures must be followed. The method described will yield a mechanically stable metallic oxide structure on the surface of the electrolyte, and will have a sintered powder formation on top of it.

Combating System Vulnerabilities Utilizing Update Expert. BRYANT FORTSON (Richard J. Daley, Chicago, Ill 60652) PAUL DOMAGALA (Argonne National Laboratory, Argonne, IL 60439).

Project Abstract Computer systems and program applications are designed with the interest of security, privacy and effectiveness in mind. Unfortunately, these designs are often initially insufficient in stopping a malicious user from destroying or gaining access to your computer. In an effort to bolster their computer systems and applications against attack, companies such as Microsoft release upgrades (known as Service Packs or Hot Fixes) to combat system infiltration due to unforeseen system vulnerabilities. These upgrades are made readily available through downloads and are dispensed to the general public and the business community alike. These upgrades in the past were generally administered on a per user basis. This method works well when faced with a small number of users on a computer network. The problem we are faced with today is how to address this type of situation for a moderate to large number of users on a computer network. This is where my project starts. I will be unveiling a new program known as Update Expert, which has been developed specifically to meet the needs of a large network. In the initial stages of this project I will be asked to develop a working understanding of how to use this program to its optimum benefit. This involves research into the companies who have already unveiled this program, the size of the networks this program has been utilized by and its possible flaws and weaknesses. In the later stages of this project I will be asked to configure and administer this program, along with troubleshooting any problems that may or may not occur.

Developing Vic and Rat replacements for use in the Access Grid. RYAN AVILES (University of Illinois at Chicago, Chicago, IL 60607) MIKE PAPKA (Argonne National Laboratory, Argonne, IL 60439).

Developing native Windows audio/video conferencing software is desirable in providing an efficient, high-quality environment for use in the Access Grid. After analyzing ConferenceXP, a partially developed conferencing application, we decided to modify its various modules where we believed were useful and recreate our own to add the functionality we believe is necessary for a high-end large-scale collaborative environment. In doing so we found that many of the modules we thought would provide us efficient solutions, in fact, did not. Mainly, the problematic areas were in the design of the application's audio/video source to network model and inability to interact with incoming streams at runtime. During our development we modified many of the capability layers in the application that were dependent on the venue web-services module for communicating with the outside venue server. This allowed us to lift a lot of CPU usage and also opened the door to creating stand-alone applications for use in the Access Grid's venue client. Furthermore, we added support for simultaneously rendering more than one camera/audio capture device. Finally, we developed various audio tools for controlling volume and developed a DirectShow filter to transform audio into 16 khz/16bit mono streams compatible with other Access Grid venue clients.

Development of a General User Interface for a Metrology Software Package to Process and Analyze Measurement Data. CHIMERE ROLAND (Chicago State University, Chicago, IL 60628) LAHSEN ASSOUFID (Argonne National Laboratory, Argonne, IL 60439).

The metrology laboratory at the Advanced Photon Source (APS),

Argonne National Laboratory, is a user facility built to characterize X-ray mirrors and other optical components for the APS user community. It is uses four different instruments (three non contact optical profiler and one atomic force microscope) housed in Class 10,000 clean room. A metrology software package is currently being developed to further process and analyze the measurement data and to generate a measurement report. This work focuses on developing a General User Interface (GUI) for the software mentioned above. The GUI is written using Igor Pro, which was also being used to develop metrology software. This report, after a brief introduction and a description of the main measurement instruments the software package, details the GUI and the obtained results.

Earned value Project Management: The Methodology and Benefits. LEONARD KENDALL (Argonne National Laboratory, Argonne, IL 60439).

Earned Value Project Management is a method used by various industries, often for software development though, for planning and tracking the cost, schedule, and technical accomplishments of a project. This methodology's main focus is on comparing the actual cost, schedule, and technical accomplishments versus their budgeted or planned budget. By using earned value a project manager is allowed the ability to predict how his or her project will perform at any stage of that project and see if at a certain point, the project is ahead of or behind schedule. Earned value has also come under scrutiny recently regarding whether or not the benefits that it provides outweigh the costs it requires. Earned value also plays a role in risk management in a product management setting by identifying threats to productivity, analyzing them, quantifying their effects, and implementing plans that counteract their effects. Earned value also relies heavily on statistical data gathering and graphing because its main purpose is to express the productivity of a project to project managers and those working on it. Data analysis and charts allow the information to be presented in a clear way that will examine the work done up the point of assessment and give clear direction on how to continue the project.

Electron Microscopy Laboratory Sample Tracking System: A Web-Based Application for Tracking Samples and Sample Analyses.

CHRISTOPHER JOHNSON (Augustana College, Rock Island, IL 61201) TANYA BARBER (Argonne National Laboratory – West, Idaho Falls, Idaho 83401)

An electronic system for storing sample and analysis information in the Electron Microscopy Lab (EML) at ANL-W (Argonne National Laboratory – West) was needed to replace an aging paper system currently in place. During the course of the appointment, a new electronic system deemed "EML Sample Tracking System" (EMLSTS) was entirely designed and implemented by the summer student. The benefits of this system include: more organized data storage, faster retrieval of information, information is more readily available for those with access, and the new system is potentially less vulnerable to data loss. The system is web-based and was written in the web language, php. It uses Oracle as a database back end. The EMLSTS was completed successfully, and at the time of this writing is being reviewed for quality assurance.

Electronic Technical Safety Requirements Tracking System. STEVEN HEMINGRAY (Michigan State University, East Lansing, MI 48825) COLIN GROVES (Argonne National Laboratory, Argonne, IL 60439).

Department of Energy regulations require Argonne National Laboratory to perform periodic maintenance on various facilities around the site. These maintenance items need to be tracked diligently to ensure that scheduled maintenance is not overlooked. Records of the maintenance need to be kept securely and accurately to have complete records of when tasks were performed and any details associated with them. This paper describes a database application programmed in Microsoft Access and Microsoft SQL Server to fulfill these requirements. The database application is in a client/server model to allow access from anywhere on the network and to facilitate database management and creating regular back-ups. This system greatly simplifies the process of tracking maintenance items, ensuring completion, and archiving the maintenance logs for later retrieval.

GeoWall Setup and its use with Access Grid Technology: Creating new Methods of Collaboration. BRIAN HLUBOCKY (University of Illinois at Urbana/Champaign, Champaign, IL 61820) MIKE PAPKA (Argonne National Laboratory, Argonne, IL 60439).

The increasing speed and decreasing cost of computers and video technology has made low-cost, passive stereo projection systems a reality. These systems are now being installed in academic institutions around the world. They consist of a computer with a dual-head video card, two LCD or DLP projectors, a polarization-preserving screen, polarizing filters, and stereo viewing glasses. Once installed, these Ge-

oWalls give scientists and students a more effective method for viewing spatially rich data sets. By combining this technology with the Access Grid™, a tool for supporting group-to-group interactions, and Access Grid-enabled applications, new forms of collaboration are created. By loading their data into the virtual venue, and launching an Access Grid-enabled application to view that data, scientists around the world can share their 3D view with each other, while discussing it using audio and video technology.

Multithreaded Sensor Server Architecture for Instrument Monitoring. OLEG YUNAKOV (*Pace University, New York, NY 10038*) GREGOR VON LASZEWSKY (*Argonne National Laboratory, Argonne, IL 60439*).

The Network for Earthquake Engineering Simulation (NEES) is a NSF sponsored nation-wide grid computing project to simulate the structural reactions to earthquakes both physically and numerically. A scaled-experiment is being conducted by Paul Hubbard in the Department of Mathematics and Computer Science at Argonne National Laboratory. The shake table and three types of sensor are used to measure building responses to the shaking. We have developed a 3D visualization software prototype in Java 3D to mimic these scaled, laboratory earthquake engineering simulations within a virtual world. This software package includes three main components: a motion control library, a set of 3D visual representation of an architectural structure, and a graphical user interface to manage and control the visual experiment. The motion control library, which can be applied to the data from a shake table, is responsible for the data representation, data streaming, building client/server environment and representing sensors. The sensor data recorded in the laboratory experiments are streamed into a server first, then forwarded to the viewer in real-time or to a data repository. Two types of data are defined in the system. One is the building configuration and sensor positioning. Each virtual sensor can self register when it is activated and be mapped onto the visual experiment. The other is the sensor motion, which is transmitted as a time-stamped multi-channel sequence.

Network for Earthquake Engineering Simulation Grid Data Acquisition Tester. JOSE CALDERON (*University of California Berkeley, Berkeley, CA 94709*) PAUL HUBBARD (*Argonne National Laboratory, Argonne, IL 60439*).

Software needs to be tested so bugs can be found before it is released and not after. Currently under development, the data acquisition (DAQ) tester is a program that is designed to test the reliability, correctness and usability of three Network for Earthquake Engineering Simulation (NEES)grid4 software components: the data acquisition system, a NEESgrid Streaming Data Server, and a NEESgrid Streaming Data Server driver. Currently, the only working test suite is the one that tests the data acquisition system. The Streaming Data Server and driver testers will be completed within two months. This paper introduces the DAQ system and explains what the DAQ tester does and how it works. The DAQ tester was developed using Java. Two reasons for choosing Java are its portability and the Swing components that are used to create graphical user interfaces (GUI). The DAQ tester tests all possible commands that the data acquisition system understands and checks that it meets the protocols, such as data format and time stamps. Because of it is a graphical user interface, one goal is to be very user friendly. Efforts have been made to accomplish this goal, such as error handling and recovery. The idea is to prevent the DAQ tester from freezing on error cases due to bad design.

Software for Reading Metabolic Reconstruction into a Database Independent Object Model. JOHN AYETTEY (*Governors State University, 1 University Park, IL 60466*) SOON OK PARK (*Argonne National Laboratory, Argonne, IL 60439*).

The field of Systems Biology builds models of biological processes based upon experimental biological data. It is anticipated that these models will grow in size and complexity as we understand more about the dynamical aspects of these systems. These models presently use data that are spread over multiple databases. These databases represent similar data in dissimilar ways. Also, the structure of the databases change over time. Dissimilar database structures makes it difficult to construct models and the evolution of the databases over time result in wasted effort maintaining applications that use the data. A database-independent object model of the biological information can be used to insulate the application from these forces. In this project, we constructed software to read data from two dissimilar Oracle databases into a common object model. We first investigated technological choices for the project, comparing ODBC based database access with Python DBI based database access. We found the Python DBI to be a much simpler, but less capable, program interface but, since it met our needs, we chose Python and Python-DBI as the technological underpinnings

for the project. We then implemented the object model in Python, wrote so-called "factories" to read data from the two databases and convert the data into instantiations of the objects in the object model. We wrote test programs and, at the end of the project, connected the software to an independently produced application that was developed in terms of the object model. This application, a Python based Model Editor, will be improved in future work to allow construction of models from data in multiple databases.

Use of Computational Methods for Functional Site Identification in the BRCA1 Protein. POUYA KHERADPOUR (*University of Illinois at Urbana-Champaign, Urbana, IL 61801*) RICHARD VILIM (*Argonne National Laboratory, Argonne, IL 60439*).

A very large protein, the human BRCA1 protein contains 1863 amino acid residues. Learning how BRCA1 interacts with other proteins would be an important step in understanding the pathology of the familial forms of breast and ovarian cancer. In an effort to reach this goal, a computational approach for finding the functional sites of the BRCA1 protein is conducted. A database of protein sequences is made either by aligning purposed domains of various BRCA1 proteins to themselves or by searching for protein regions similar to the BRCA1 domains. Because of the importance of the functional sites to proteins they, like amino acids involved in protein folding, are preserved evolutionarily. However, unlike fold related positions, functional sites may not be preserved in structurally similar yet functionally dissimilar proteins. Thus, we seek positions that are preserved through protein sequences of the same class yet not preserved in protein sequences over all sequences in the database. This is done through using methods that were developed for protein classification. Either we assign scores to each position using a method involving the direct variability of a position among sequences, a log odds ratio similar to those used to generate the BLOSUM substitution matrices, or by using a genetic algorithm designed to classify proteins. These scores can be used to identify potential locations for a functional site. Unfortunately, the results were not as favorable as we had hoped. The BRCA1 domains had too little homology to be properly compared, thus generating a database by aligning BRCA1 domains to itself was ruled out. Further, only one domain of the BRCA1 proteins, R1, had sufficient homology in the NCBI protein database to allow for comparison of BRCA1 with other proteins classes. Results on it are pending additional investigation although are initially promising.

Work with the 2-ID-B Intermediate-energy Scanning X-ray Microscope at the Advanced Photon Source. NATHAN KRAPP (*University of Chicago, Chicago, IL 60637*) IAN MCNULTY (*Argonne National Laboratory, Argonne, IL 60439*).

The 2-ID-B beam line at the Advanced Photon Source (APS) at Argonne National Laboratory (ANL) is dedicated to providing users X-rays in the 0.64-4.0 keV range, usually for scanning transmission/fluorescence X-ray microscopy and coherent X-ray scattering. The work done over the summer of 2003 has improved the ability of 2-ID-B to meet the needs of visiting scientists, by providing a new arrange of procedures written in the IDL language, providing experimental control and analysis for a variety of different tasks, including scanning X-ray microscopy, coherence measurements, holography, and phase detection. Work was also done ascertaining the modulation transfer function (MTF) for the scanning X-ray microscope at the station. It was found that the MTF is very close to the ideal, providing good transmission power at almost all attainable resolutions. The notable exception occurred at a spatial frequencies near 8 \mu m^{-1} , which is the zone plate limited optical resolution as determined by the Rayleigh criterion. More work will be done with the MTF in the future, using different zone plates in order to create varying limited optical resolutions, and also using scanning electron micrographs to provide more accurate input images.

Automating Pivot Table Generation for Microsoft Excel Using SQR, VBScript, and COM. CHRISTOPHER SIMPKINS (*Community College of Rhode Island, Warwick, RI 02886*) GREGORY MACK (*Brookhaven National Laboratory, Upton, NY 11973*).

The Business Systems Division is responsible for creating Budget and Expense Reports that are used throughout the laboratory for financial design and analysis. These reports must provide data that is clear and concise. One way to present data in such a manner is through the use of pivot tables in Microsoft Excel. Pivot tables allow for dynamic, run-time data analysis and ad-hoc formatting. By automating the generation of pivot tables, the confusing and time-consuming process of manually creating them may be eliminated. This project is written using SQR (Structured Query Report Writer), VBScript, and COM (Microsoft Component Object Model). The data used for the Pivot Tables is pulled from an Oracle database and passed to the generator through an existing SQR program. Since the native Microsoft Excel Workbook (XLS) file format is proprietary, the Excel files are output in web page format. Mac-

ros are generated dynamically as VBScript. These macros utilize COM to run against the Excel file and create pivot tables based on options specified through a PeopleSoft front-end.

Cyber Security on a Local Network Server & Microsoft Access Database Conversion. CHERYL BROWN (*Borough of Manhattan Community College, Manhattan, NY 10007*) PATRICIA WILLIAMS (*Brookhaven National Laboratory, Upton, NY 11973*).

The objective of this paper is to apply practical theory of Microsoft (MS) Access in transitioning Access 97 to Access 2000. This research assignment will be conducted at Brookhaven National Laboratory's (BNL) Facilities and Operations Directorate. The result of this transition is to analyze what occurs to some of Access 97's databases when they are transferred over to Access 2000, which cause some missing/erroneous data. The significance of tracing missing/erroneous data is important since the majority of databases contain macros that execute various functions on Directorate training, injury and contractor programs, as well as other unclassified and miscellaneous documents. In conjunction with troubleshooting MS Access' data, the procedures of developing a Cyber Security for the Directorates server will be integrated into this project. Due to the importance of scientific and technical research conducted for the United States Department of Energy at BNL, there are literally thousands of daily cyber attacks to their network system. As a result of these cyber attacks, the Framework of Database Security at BNL entails encrypted data, which is protected from any unauthorized disclosure (Cyber Attacks includes Computer Hacking, Cyber-Terrorism (Viruses) and Patent and Trade Mark Theft). Certain procedures must be formatted before setting up a local server which contains databases and other important records. Limited access and password information, being the first two processes begins from creating exclusive rights, to finalizing on the database. It must also be noted that the importance of the database itself is placing certain authorized information for BNL employees to have entitled access features.

Data Management and Compression at PHENIX. LUKE ST. CLAIR (*University of Illinois at Urbana-Champaign, Champaign, IL 61820*) BRANT JOHNSON (*Brookhaven National Laboratory, Upton, NY 11973*).

In the last few decades, the amount of information collected at the biggest of the big physics experiments has surged from gigabytes to terabytes to petabytes, emphasizing the experiments' need for effective data management and compression. Data retrieval, management, and presentation: The purpose of the research into better data management and accessibility was to enable the collaborators at RHIC to easily access different slices of datasets in the form of useful summaries and search results. In order to manage personnel data, speaker nominations, records of talks, etc., a system of PHP-generated web pages was designed to interface with a MySQL database. Updating the database, submitting new information, and searching were all implemented in web-based utilities, with appropriate permissions added. These pages were specifically designed to utilize certain chunks of code repeatedly in order to allow the code to be used in a wide variety of applications. In addition, pages were generated to allow users of the data carousel to easily and graphically check on both the status of the carousel and the status of their job submissions. PHP, coupled with MySQL queries, automated many complicated and commonly-performed searches of data carousel information, as well as added new data groupings and the ability to predict the delivery time of files. The result of these projects is that users can now manage and interpret existing sets of PHENIX data without any additional training. Data Transmission and Compression: In order to save results from PHENIX, event data comes from computers that collect the data and goes to buffer boxes which store and then export the data for permanent storage. The compression between the ATP computers that send this data and the buffer boxes was investigated in the hopes that more PHENIX data could be saved in the future, instead of throwing away data that initially looks uninteresting. The gzip algorithm was previously used to compress data from the ATPs, and code was written to test the its capability against the speed of the LZO family of algorithms and the better-known bzip2 compression. LZO compression was shown to be faster in every test performed, though it affords ~10% less compression. However, with the addition of two more buffer boxes, tests suggest that LZO compression could sharply increase the amount of data transferable, which should allow PHENIX to store even more data in the future.

Designing and Testing Applications using PeopleSoft. EDGAR MANIEGO (*Borough of Manhattan Community College, New York, NY 10007*) MARIE VAN BUREN (*Brookhaven National Laboratory, Upton, NY 11973*).

The Business Systems Division (BSD) of Brookhaven National Laboratory is responsible for maintaining records of the training courses and

requirements that each employee and student needs to take. One of the uses of these records is for security and safety reasons. These reports and data are stored in a database system for manipulation and easier data selection. BSD uses PeopleSoft, which interacts with Oracle, BSD's chosen database system, to run and control their data. In addition, BSD uses SQR (Structured Query Report Writer) and SQL (Structured Query Language) to process and retrieve data from Oracle. SQR works with many popular database systems. PeopleSoft is a software environment that let us create, design, and test reports, tables and pages in an easier manner. It also incorporates security so data is protected and can only be accessed by certain people. Reports, tables, pages, and menus are created, tested, and incorporated into a website for the user using PeopleSoft, to display outstanding training courses.

Developing Calibration Procedures for a Low-Cost Temperature and Relative Humidity Transmitter. JENNY KIM (*Rensselaer Polytechnic Institute, Troy, NY 12180*) R. MICHAEL REYNOLDS (*Brookhaven National Laboratory, Upton, NY 11973*).

This paper describes the best method for calibration of the low-cost Temperature and Relative Humidity (T-RH) probes that will be used in the new heated Free-Air CO₂ Enrichment (FACE) experiments. The goal was to be able to calibrate these probes to 0.1°C accuracy by simply applying the mean offset and avoid the complexity of performing a linear or higher-order regression. Ten pre-assembled probes with Thermo metrics® RL1005 thermistors and Atmel® AVR microprocessors were placed in an environmental chamber with accurate references for the calibration test and the resulting data were analyzed using procedures developed in Mat lab®. Once the mean was taken of the probes? Most stable readings, these values were tested for their validity against the reference temperature values to determine if they satisfy the condition for an offset correction. Having concluded this, the offsets were applied to the existing values and the mean of the probes' corrected temperatures was computed at each stable point. These values were then compared with those of the reference to determine whether an accuracy of 0.1°C was achieved. Results showed that the responses of the probes were quite satisfactory given their low cost. Also satisfactory was the level of accuracy achieved in the calibration test, with a standard deviation of less than 0.1°C. Given these results, further testing will be performed on more of these T-RH sensors with confidence that the outcome will agree as well as they have in this case.

Evaluation and Implementation of Big Brother® Network Monitor System. JOSE PEREZ (*Hostos Community College, Bronx, NY 10451*) KEITH LALLY (*Brookhaven National Laboratory, Upton, NY 11973*).

With the technological advances in information technology systems and related applications, the demand for improved methods of monitoring and supporting these systems has increased. Big Brother® is a network monitoring program that enables system administrators to obtain real time information about processes running in different computer systems. This information is gathered in central location in which the data can be later evaluated. Having the ability to visualize and analyze problems from a central point decreases the downtime in crucial network services and decreases the related costs of technical support. In addition, problems with network services and network applications can be corrected before the end users see any interruption in their normal network activities. This paper tries to determine if Big Brother software is able to deliver the right tools to monitor crucial database applications, internet related services, local machines applications and resources. At the same time, Big Brother must be able to present a clear interpretation of the status of these services in real-time. This evaluation of Big Brother goes from the requirements of the software to the actual implementation of it on a bigger scale. The results obtained in this research show the versatility of Big Brother to monitor small and mid-size networks environments, but also show some deficiencies when more complex monitoring features are required, which are needed in big-size enterprise systems.

Installation and Configuration of Portable Batch System (PBS) and Ganglia onto a Server for the Use of the Grid. PAUL FUREY (*State University of New York New Paltz, New Paltz, NY 12561*) EDWARD MCFADDEN (*Brookhaven National Laboratory, Upton, NY 11973*).

Scientists have limited resources at their disposal but with today's technology it is possible to supply as many people as possible with as much power as necessary. This particular task is a small part in the massive Grid Project. We set out to install and configure the different programs that are used to monitor computer servers. The specific computer server that was worked on in this task was a small four-node Red Hat Linux server.

Programming for Madout and Magnet Files. AMIT KAPOOR (*New Jersey Institute of Technology, Newark, NJ 07102*) JORG KEWISCH (*Brookhaven National Laboratory, Upton, NY 11973*).

Programming is a way to interact with computers and solving several intricate problems. A programming language is a tool used by programmer to interact with computer. Program solving involves two steps: first step is, analyzing the problem by understanding the problems and its requirements. Second step is, developing a solution by writing procedures (an algorithm). For example, programming for madout files and magnet files. The main reason behind the programs was to give output of the files as efficient as possible. A user can acknowledge all the important information without opening a certain file. Moreover, a user can view various files at a same time. Using the programs for madout and magnet files, a user can compare data as uncomplicated and straightforward, as a result of this user would save ample of time.

Scatter Correction in the Micro PET R4. TIMOFEI GERASIMOV (*Harvard University, Cambridge, MA 02138*) DAVID ALEXOFF (*Brookhaven National Laboratory, Upton, NY 11973*).

Photon scatter and attenuation are important confounding factors of quantitation and image contrast and detail in the Concorde Microsystems [CMS] Micro PET R4, as in all PET cameras. Until relatively recently, there has not been a standard method of scatter or attenuation correction for this camera. The purpose of this study was to quantitatively evaluate, in both sinogram and image space, the following: scatter correction by fitting a smooth curve to the emission tails, and CMS's own single-scatter simulation- [SSS] based scatter correction; and CMS's transmission-based attenuation correction. In order to study the effects of scatter and attenuation correction on objects with varying geometries, we constructed and scanned 3 different phantoms: two "slot" phantoms with surrounding scatter media (phantoms 1 and 2), and a "cold rod" phantom (phantom 3). For each phantom, we performed an emission scan and a transmission scan. The transmission scans were smoothed and segmented in image space to produce the most accurate possible attenuation maps for SSS and attenuation correction. After normalization, emission scans were scatter corrected using no scatter correction, fitting a quadratic and a Gaussian curve to the profile tails, and SSS. Each resulting sinogram was then reconstructed both with and without attenuation correction applied. In both sinogram space and image space, we used a ratio of the counts within a known cold region to that within a known hot region, as well as ratios between two regions with different, known amounts of activity. These ratios were computed for each combination of scatter correction and attenuation correction described above. In every case, SSS correction performed better than fitting and a Gaussian performed better than a quadratic. Attenuation correction worsened quantitation, but was seen to improve image quality significantly in Phantom 1, and somewhat so in Phantom 3. We conclude that the SSS algorithm, when supplied with an accurate attenuation map, is superior to both quadratic and Gaussian fitting as a method of scatter correction. However, the high performance of the Gaussian fit combined with its superior speed and no need of an attenuation map also makes it a good choice for routine scatter correction. We believe that attenuation correction, while having a consistently adverse effect on quantitative measures, is necessary for accurate image processing because of its effect on image quality.

Stereographic Visualization of Scientific Data Using Commodity Hardware. BRIAN ROWE (*Jamestown Community College, Jamestown, NY 14701*) BRIAN ROWE (*Brookhaven National Laboratory, Upton, NY 11973*).

Currently Brookhaven National Laboratories uses large, proprietary hardware in their Stereographic Visualization Theater. We have ported the theater's software to work on commodity hardware. We initially tried to use the Microsoft Windows 2000 operating system, but due to issues involving interprocess communication, we decided to use Linux. The switch has reduced overall system cost, and by reducing physical size, it has made it easier to participate in trade shows.

Three Dimensional Visualization Software. RONALD HUEGEL (*Alfred State College, Alfred, NY 14802*) CARMEN BENKOVITZ (*Brookhaven National Laboratory, Upton, NY 11973*).

Research cont. from 2002. Visualization software is helping doctors and scientists save not only lives but also the Earth. 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. There are currently a couple versions of Vis5D available, Vis5D+ and vis5d-5.0. We explored/tested the different versions of Vis5D, and various hardware and software platforms to determine which one is best for our data and computing needs. 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). Therefore, it has been necessary to use two working versions for our experiments. Vis5D+ is the most recent version it does however some of its features are not compatible with SGI machines on which we are running the visualization experiments. We have downloaded and compiled an earlier version Vis5D-5.0, just in case it might be needed. Despite some technical difficulties, Vis5d has proved to be a flexible and powerful tool for visualizing MOPUT data.

Comparing Classic Intrusion Detection Test Data Against Data Found In The Wild . MATTHEW MORGAN (*University of Tulsa, Tulsa, OK 74104*) HOWARD WALTER (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

With the impromptu development and heterogeneity of today's Internet, things don't always go as planned. Real-world Internet traffic exhibits far more variation than is generally appreciated by the application development community. Poorly configured routers, faulty software and many other factors can maim packets, destroying the information they contain and confusing the applications that receive them. Unfortunately, network security applications are no exception; intrusion detection systems (IDSs) developed and tested in controlled environments tend to misbehave when exposed to unregulated traffic on the Internet. This paper will compare inconsistencies in network traffic protocols between synthetic and raw Internet data using the Bro intrusion detection system. Differences between 'classic' synthetic data and 'raw' Internet traffic will be enumerated and used to explain why applications tested only with synthetic data tend to fail when placed in the real world.

Computer-Aided Learning of Building Controls. CLINT JOHNS (*University of California, Davis, Davis, CA 95616*) PHILIP HAVES (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

As California's population increases, so does the demand for energy consumption. However, as power plants and alternative energy sources attempt to keep up with the demand, they are still not producing enough energy. A research group at Lawrence Berkeley National Laboratory has invested an interest in conserving California's energy. In particular, their research focuses on one of the biggest energy consuming industries, namely large commercial buildings. One strand of research is to create a vocational program to teach building operators and technicians how to operate and maintain their buildings more efficiently. In order to realize this project to fruition, a proof-of-concept study along with proposed curriculum is being created to submit to NSF for funding. The study is one proposed lesson that uses a prototype learning tool, allowing a user to operate the controls of a simulated building. The learning tool runs a simulation program, SPARK, while presenting a user-friendly interface. The simulation program can emulate any combination and any type of building controls. The interface is being created with the target audience, technicians, in mind. Before practicing with real controls, the simulated learning environment will be the testing ground for building operators and technicians. Issues being explored vary from how the interface will communicate to SPARK, to the look and feel of the interface, to how portable the solution should be. This document explains the first steps in the design of a prototype learning tool for the proof-of-concept study along with preliminary results.

Execution Flow Internals of a Parallel Job Using LAM/MPI 7.0. VIKRUM NIJJAR (*Mission College, Santa Clara, CA 95040*) CHARLES VERBOOM (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

Local Area Multicomputer (LAM) is a widely used open-source implementation of the Message Passing Interface (MPI) specification. Its stability and rich feature set coupled with the open-source model it follows makes it an attractive candidate for use on Beowulf-class scientific clusters. As the deployment base grows and the code matures, details such as architectural design and execution flow are hidden deeper behind layers of abstraction from users interested in learning of these internals. This paper examines the execution flow of a simple parallel job being run across a LAM/MPI environment.

Linux, Tomcat, and MySQL: An Open Source Makeover for the EPA's Home Energy Advisor. BRADFORD WILSON (*City College, San Francisco, San Francisco, CA 94112*) RICH BROWN (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

The Energy End-Use Forecasting (EUF) group at Lawrence Berkeley National Laboratory provides the EPA's Energy Star program with a va-

riety of energy analysis tools and reference reports. One such tool is the Home Energy Advisor, a second-generation web application designed to help homeowners reduce energy use in their homes. By entering a zip code and answering a few questions about their home's construction, orientation, and major appliances, users can quickly identify the best energy upgrades for their home and view potential energy savings from these upgrades. Behind the scenes, Advisor performs a zip-code lookup of relevant climate and energy market data in its database. Total home energy use is then calculated in real-time using sophisticated models and data developed at Berkeley Lab, most notably the DOE-2 building simulation model for heating and cooling. Advisor was originally implemented in Tango, an early web development environment. As the web site grew in popularity, the application was unable to scale to meet demand, and a new software architecture was needed. The decision was made to port (re-design) the application to Java technology. The outcome of this effort is a Java Enterprise Edition (J2EE) web application using Enterprise Java Beans (EJB's) running on BEA WebLogic server with an Oracle database. This architecture is considerably more ambitious than the Tango version, and as such requires a proportionally greater investment in technology and personnel to maintain it. Unfortunately, funding for Advisor has all but slowed to a trickle, leaving the project in crisis. My research focused on developing a plan to reduce fixed operating costs associated with Advisor, to reduce complexity in the application architecture, while simultaneously increasing performance. The reduction in operating costs is achieved by replacing expensive proprietary server software with well-supported open source equivalents. Proposed changes to the architecture include eliminating EJB components, replacing WebLogic server with Apache Tomcat, and switching from an Oracle database server to a Linux-based MySQL server. Anticipated performance benefits come from eliminating overhead associated with EJBs, and streamlining object/database mapping operations. This plan will save over \$15k/year in licensing and hosting fees, and may significantly reduce future development and maintenance costs.

Password Security. BONNIE CHANTAROTWONG (*Contra Costa College, San Pablo, CA 9480394803*) TOM MURPHY (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

We rely on password for so many things: bank accounts, airline tickets, email, computer logins, and web pages, just to name a few. Yet few of us really understand the methods by which our passwords are protecting us, and even less understand their vulnerabilities. Educating computer users of the necessity and methods for creating secure passwords is perhaps the most beneficial form of security for the least monetary cost. Yet, surprisingly, the vast majority of computer users have no idea of what constitutes a reliable password. Besides this lack of user understanding, password cracking has become an increasingly attractive break-in method for several reasons: machines are becoming faster and cheaper, cryptographers are finding more efficient cracking algorithms and optimizations, and machines can be networked together, resulting in powerful parallel computing. For these reasons, it is important now more than ever to educate the public of password security. For this project, I have researched topics such as: how passwords are encrypted, how password crackers work, the difference between various cracking modes, what constitutes a good password, and the ethical and legal complications of password cracking. I also installed and ran a password cracker, John the Ripper, on various encrypted password files to test how different factors—such as length, complexity, and predictability—affect crack time. My experiments were run on user passwords encrypted with the standard UNIX crypt() function. My research reports the algorithms by which many password crackers operate, as well as the results of my controlled experiments. From the gathered data, we can quantify the improvement resulting from longer, more complex, and unpredictable passwords.

The Future Advancements of SAN I/O and Transfer Technology. ELGIN AMBOREE (*Texas Southern University, Houston, TX 77004*) REI LEE (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*). SAN Fabric I/O and Storage Transfer Technologies have been used in HPC world for many different applications; from the most common Fiber Channel Switches, to the more discrete uses of 64 bit microprocessors. These varieties of uses are what make these technologies a popular field of study. As scientist we are devoted to improving the scalability of the I/O technologies. For example, these technologies have been used to make the microprocessors 4 times as fast. This prevents the scientist from having to wait all day for the results of a scientific experiment. These are not the only things that this technology can be used for, however. San Fabric I/O and Storage Transfer Technologies can also be used for Global Unified I/O and Storage Control other wise known as a Global Shared-Disk system. The basic objective is to study the peak

performance of the Disk-System under extreme conditions. For the extreme test we have chosen the iSCSI protocol for I/O benchmarks. The ideal iSCSI card would hopefully put out about 100 Mb/s. This would lead to much faster I/O rather than using regular disk systems. The iSCSI technology is still young and in order to manipulate it we are going to need to do many benchmarks to test its scalability against GUPFS.

Tuning Oracle 9i. ROBERT KELBLEY (*Ohio Northern University, Ada, OH 45810*) CLAYTON BAGWELL (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

The emergence of cost effective servers using open source software and 32-bit x86 based hardware allows for a reliable and inexpensive server environment. Running proprietary database servers, specifically Oracle, on these systems provides relational database opportunities and performance that was previously only available on high-end proprietary servers. The flexibility these setups provide allows considerable tweaking at the hardware, operating system, and database level. When database performance starts to degrade because of increasing data amounts, user activity, and database complexity, the cause of the performance degradation can be elusive. Database administrators running Oracle on open source distributions, most commonly Linux, must prevent database bottlenecks which decrease the performance of applications dependent on those databases, especially for Online Transaction Processing (OLTP) web applications. Much research has been done and documented in technical papers and books on setting up efficient Oracle servers on Linux and also Oracle optimization techniques. An outline of some critical parts of Oracle database tuning was created from all of this information. First, it is important databases are set up using available performance enhancing options. Next, the different memory areas Oracle uses must be optimally configured. Finally, slow queries should use techniques available to improve performance when possible. Different options available include using materialized views in place of dynamic views, adding indexes, and using cursor sharing.

Creation of a Computerized Interface to Control the 3M Thin Film Deposition System Using Lab VIEW. EDUARDO MOUTINHO (*Colorado School of Mines, Golden, CO 80127*) 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 creating such a program to control the 3M Thin Film Deposition System.

Solar Radiation Data Quality Assessment Software Upgrade. JEREMY COOK (*University of Kansas, Lawrence, KS 66045*) STEPHEN WILCOX (*National Renewable Energy Laboratory, Golden, CO 89401*).

Solar radiation measurement is an important part of solar resource assessment, as the world continues to look to the sun as a source of clean, renewable energy. Critical to accurate solar radiation measurement is good assessment of data quality. The National Renewable Energy Laboratory (NREL) has an automated quality assessment software package, known as SERI QC, to aid in quality assessment of data. A vital part of this package, QC Fit is a boundary fitting tool enabling the analyst to interactively set expected values. Advancements in computer technology have made possible the desire to update QC Fit and expand on its capabilities. By porting the program to the Microsoft Windows platform, QC Fit has been vastly improved. It is now easier to use due to the graphical nature of Windows, and aids the analyst in setting boundaries more quickly and accurately.

Aqua Sentinel: Working for Homeland Security. DAVID FEAKER (*Tennessee Technological University, Cookeville, TN 38505*) DAVID E. HILL (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The Aqua Sentinel project, designed by Dr. Elias Greenbaum and Charlene Sanders and receiving help from Miguel Rodriguez and Dave Hill at the Oak Ridge National Laboratory, is a United Defense funded program for Homeland Security. The present project involves designing a program, AquaData Interpreter, for the United Defense Aqua Sentinel

project. Aqua Sentinel is a newly patented bio-terrorism defense technology. This technique works by comparing the fluorescence given off by algae that is naturally present in a healthy drinking water supply with the fluorescence of drinking water that has been poisoned with a toxin like cyanide. Through the use of this program, one can determine whether or not the water is safe to drink or can potentially pose a health risk. The AquaData Interpreter is a computer program designed in C/C++ which takes the measured fluorescence data and compares the healthy sample to the sick sample. By comparing the variances of each data point corresponding to time in seconds, a chart can be created to show the significant differences between healthy algae and poisoned algae. It was found, through the use of the AquaData Interpreter program, that with even a small amount of poison, a big effect can be seen in the health of the algae. Thus by having the technology to detect harmful substances before the water is taken into a filtration system, disaster can inevitably be averted.

Construction of a Three-Dimensional Bifurcation Model for Lung Airways. ERICA SHERRITZE (*Tennessee Technological University, Cookeville, TN 38505*) RICHARD C. WARD (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

A graphical, three-dimensional model of the lung airway is the first step toward a goal of studying the effects of environmental toxicants or therapeutic aerosols on the human body. In order to develop this geometric model, a numerical investigation of the mathematic equations used to construct a previous model* was conducted. Using these equations and the given symmetric parameters, a copy of the model was generated. This first step involved using symbolic computational software, Maple 8, to simplify the equations. Once simplified, the equations were incorporated into a Microsoft Visual Studio C++ program to generate sets of points which were imported into Rhinoceros 3D NURBS Modeling program. Non-Uniform Rational B-Splines, or NURBS, are vector-valued piecewise rational polynomial functions that are used as a geometric tool for computer-aided design. After each equation was transferred into Rhino 3D, the process of constructing a three-dimensional model from the two-dimensional curves began. Curves located in the x, y-plane were then lofted with curves located in the x, z-plane to create the circular, parent segment of the bifurcation. Similar procedures were performed to create the remaining daughter branches and flow divider portions of the bifurcation. The result was a symmetric three-dimensional model of a lung bifurcation. Having this example model will enable slightly more realistic, future designs with asymmetric and multi-planed branching, to emerge through the alteration of the beginning equations and parameters. Multiple branches will then be scaled and added to the model to replicate the airways in the lungs. These designs will also be used to fit real CT data taken from the airways of pigs and humans. This work is a small portion of a much larger research project to develop a virtual model of the human body.

Displaying Oceanographic Data with The Live Access Server.

TIMOTHY RACZ (*Appalachian State University, Boone, NC 28608*) ALEX KOZYR (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*). Data visualization is helpful for finding interesting features in data and for formulating hypotheses. To make data visualization possible over the internet, the Thermal Modeling and Analysis Project (TMAP) at the Pacific Marine Environmental Laboratory (PMEL) developed the Live Access Server (LAS). This configurable web server, along with a visualization application known as Ferret, allows access to geo-referenced scientific data and can produce various types of color-coded maps, graphs, and plots of the data. These features make LAS suitable for use with oceanographic data gathered by the Carbon Dioxide Analysis Information Center (CDIAC). While the LAS software is capable of handling gridded oceanographic data derived from original bottle measurements, it has no means of handling the bottle measurements. Effort has been spent on customizing LAS's ability to reference this raw bottle data. This requires writing a program that converts the bottle data into a form LAS can handle. Another problem is to configure LAS to depict sampling stations on the maps that are produced from the gridded data. This can be accomplished by writing custom scripts that are used by the Ferret data visualization software. While bottle data access has been successful the display of sampling stations has not yet been accomplished. The LAS software is quite flexible and allows data providers to customize it in many ways. LAS allows web users to obtain the data they need in a variety of different formats making the data easier to interpret. Displaying oceanographic data with LAS provides a powerful tool for anyone who needs to access this kind of data.

Information Analysis Techniques Using Upper Ontology Languages. TRAVIS BREAU (*University of Oregon, Eugene, OR 97403*) THOMAS E. POTOK (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

With increasingly ubiquitous networks has come an unprecedented flow of digital information. The tools to analyze (i.e., manage, evaluate, classify) and visualize (i.e., search, retrieve, present) information from multiple, inhomogeneous sources have largely relied on improvements in statistical methods. The results from statistical methods, however, significantly overlook the relevance of semantic features present within natural language and text-based information. Emerging research and development in ontology languages (e.g. RDF, RDFS, SUO-KIF, and OWL) offers promising avenues for overcoming the limitations inherent in statistical methods by leveraging existing and future libraries of meta-data and semantic mark-up. Using semantic features (e.g. hypernyms, meronyms, synonyms, etc.) commonly represented in ontology languages, subsumption inference can be used to reason about document content at conceptually higher levels than statistical methods. Subsumption inference fundamentally provides the capability to traverse class hierarchies composed of predicates, or in this case, words from natural language. This paper begins with a background in contemporary statistical methods required to introduce an alternative classification and search algorithm using semantic features commonly found in ontology languages. Following is an overview of eight popular ontologies, both dictionary and inference-based with attention to features desirable for use in the specified algorithm. In addition, the results from the search algorithm and companion software tool that uses Princeton University's WordNet as the ontology for searching text documents is presented. As one of the eight ontologies reviewed and the largest, most comprehensive dictionary-based ontologies, WordNet is attractive for evaluation purposes and prototyping. Finally, from problems discovered in both dictionary and inference-based ontologies, a set of guidelines are presented for evaluating and/or developing ontologies for use in the stated algorithm.

National Energy Assurance Analysis Center. KIMBERLY WINDOM (*Robeson Community College, Lumberton, NC 28358*) ANDREW S LOEBL (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Oak Ridge National Laboratory (ORNL) has proposed to the Department of Energy (DOE) and its Office of Energy Assurance (OEA) to establish an advanced computationally based non-classified, collaborative environment called the National Energy Assurance Analysis Center (NEAAC). The goal of NEAAC is to generate, integrate and provide enabling data, systems and technologies that will assure the DOE and its collaborating organizations and agencies-federal, state, or local-the continuity and viability of our nation's critical energy infrastructures, which, along with the other critical national infrastructures, provide the essential services that support the operation of our society. NEAAC's objective is to ensure a secure and reliable flow of energy to America's homes, industries, public service facilities, and transportation systems. To accomplish this there is a need for close collaboration with the private sector. NEAAC is needed in collaboration with the OEA to identify critical infrastructure components and interdependencies, identify natural and malevolent threats to the infrastructure, recommend actions to correct or mitigate infrastructure vulnerabilities, and plan for and provide technical support during emergency response and other system disruptions. The collaboration offered in the proposal currently consists of two National Laboratories, ten Universities with specialties spanning the entire energy supply and distribution sector in the U.S., including Oak Ridge Associated Universities (ORAU). Each institution is respectively affiliated with regional and local energy suppliers/distributors. This collaboration is the basis upon which analytical methods, new knowledge and computer based tools in a hosted collaborative research and training virtual environment will be developed under NEAAC. The students' summer assignment has focused upon the computational science and computer/network specifications by which open and effective Research and Development Programs can be accomplished. To better document the specifications of the network bandwidth, software technologies, mass storage, and visualization capabilities available through ORNL's advanced computational resources, research and interviews are in progress so that current technology can be documented to better understand how to create that advanced collaborative environment, envisioned through NEAAC, for the benefit of DOE and its missions.

The Genetic Algorithm as a Means of Modeling Electrical Power Generation Levels. JENNIFER CAMP (*Purdue University, West Lafayette, IN 47907*) VICKIE E. LYNCH (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Computer simulations to predict the cost and availability of electricity could be very helpful as the power industry is further deregulated. To most accurately reflect the electrical generation of utility companies, the simulation must employ a form of artificial intelligence in order to learn the most effective generation strategies. The genetic algorithm is used to simulate the learning techniques of the utility companies, which are

represented as intelligent agent objects. Based on the total expected demand and a set of predetermined rules, each agent decides upon a bid of how much electricity to generate. The chromosomes of the genetic algorithm represent what rules the agent is currently utilizing to determine the bid. After the bids are made, a decision is made on which bids to accept based on a realistic modeling of the electric grid. After the power is dispatched, the agents are then informed of the amount of their electricity that was actually used and the price that was paid for the electricity. Using these results, the chromosomes are then manipulated using the standard reproduction, crossover, and mutation procedures of the genetic algorithm. One would expect the agent's generation levels to organize to a point where each agent was earning the maximum profit. The final version of the simulation showed evidence that the agents were learning and that the generation levels were organizing near the expected values given by the economic models. Current research is being performed to merge this simulation with an existing simulation that models power transmissions in a given network. In this code, power is dispatched using power flow equations with linear programming, and the agents represent the utility companies associated with the generator nodes of the network. The agents must adjust their levels of generation to the changes in demand and the amount of power that can be transmitted on the lines of the grid. Initial results of the coupled codes show good agreement with the economic models.

Three Dimensional Data Visualization Using the Visualization Toolkit. ERIC MUELLER (University of Tennessee, Knoxville, TN 37996) ROBERT HARRISON (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

VTK, the Visualization Toolkit, is a powerful and comprehensive open-source tool for the visualization of data. Unfortunately, VTK is a programming interface rather than an end-user program, and using it directly to visualize data, though not overly painful, requires more time than can be afforded. To handle this problem, data-viewing applications are designed, usually for particular uses. One such use is in the visualizations of the higher-dimensional data sets which may be generated by approximating solutions to the electric potential equations in a molecule. Although the data is of course significant, a grasp of the processes used to generate the data is not necessary for the understanding of such a visualization utility. Current programs designed for use in this type of visualization, such as ParaView and MayaVi, are complex and counter-intuitive, as well as being very restrictive of the types of data that may be displayed and manipulated. New applications must be developed for the particular requirements of these data sets.

Using Concepts of E-Commerce in Scientific Data Applications- Atmospheric Data. CORTEZ HARVEY (DePaul University, Chicago, IL 60604) RICHARD WARD (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The Atmospheric Radiation Measurement (ARM) archive contains ten years worth of atmospheric data including microwave, radar, lidar, and energy flux measurements in NetCDF format stored on the High Performance Storage System (HPSS) at ORNL. Links to the ARM data are maintained as metadata in a Sybase database. A user interface is being developed to allow users quick access to the ARM data via the metadata links. This interface essentially mimics E-commerce in that it provides the user opportunities to view metadata and order data in a manner similar to ordering products on the Internet. The user first selects a site, facility, instrument, month, and year for the desired data. Thumbnails (or miniature plots) corresponding to the data matching the selection criteria are displayed for each day of the selected month. The user selects a day by selecting a thumbnail. A set of plots for the primary measurements of the selected instrument is then displayed. This set of plots is referred to as "quicklook" plots because they give a quick view of the raw data in the ARM archive. This project uses a technology called Java Server Pages (JSP) and Java Servlets to implement the process of viewing information and ordering the data. Developed on a desktop PC, the application has been ported to the development server in the Environmental Sciences Division, where it will serve as the prototype for the ARM data "quicklook" browser.

Value Chain Analysis Application. JOHN KNOX (Roane State Community College, Oak Ridge, TN 37830) RICHARD WARD (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The Value Chain Analysis (VCA) method has been applied to aid steel manufacturers in finding the most productive way of making their products while minimizing their cost. A computer application using the VCA method was developed in Microsoft Access to allow the user to input initial data ranging from raw material to variable costs and to enable tracking of specific information as material is passed from one process to another. The Microsoft Access VCA application has been completely rewritten to improve the user interface and clean up the

database design. With the new version, the user can view sensitivities (e.g., rate of change in product produced per rate of change in energy consumed) and the effects of incorporating new technologies. At the moment, optimization of the technology analysis is done in the MATLAB environment, but soon these calculations will be integrated into the new VCA application. Instead of using Microsoft Excel to generate plots and graphs, they are now done in Microsoft Access which is leading us towards our goal of having the entire program contained in Microsoft Access. We're designing the new VCA application to be flexible enough for use in other optimization problems. An example of this is the use of wireless technology in monitoring industrial processes.

Visualization of Scientific Data over Wide Area Networks. KAYA SHAH (Massachusetts Institute of Technology, Boston, MA 02139) S. V. NAGESWARA RAO (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

In today's world of advanced computing, data modeling is taking on a new role of importance. Scientists generate large, multidimensional data sets through simulations, experiments and computations. Furthermore, these data sets are rapidly gaining in size. When terabyte data sets need to be analyzed, terascale computing is necessary. Most scientists do not have local access to terascale computing power and thus access supercomputers over networks. This paper examines the process of visualizing three-dimensional scientific data over a network. In order to explore the actual visualization process, interpreters, visualization toolkits, and software programs were familiarized with. Interpreter languages such as Tcl/TK allowed programming in the Visualization Toolkit (VTK). Additionally, experiments were conducted with ParaView and MayaVi, which are visualization programs that run on top of VTK. To better understand the flexibility of ParaView, filters and modules were added to the program by modifying the source code. In order to explore visualization over networks, communication between two computers on a LAN was achieved through sockets. The next steps involved writing a program to compare data set size and transmission time as well as make the decision to visualize the data set locally or remotely. Future extensions of this project include experimentation over a globally distributed test-bed for network services, such as PlanetLab.

Automation of Atmospheric Radiation Measurement Program's Data Object Design Web Page Using PERL Scripts, XML and PHP. CARRIE VALATKA (University of Toledo, Toledo, OH 43606) MATTHEW DONNELLY (Pacific Northwest National Laboratory, Richland, WA 99352).

The Atmospheric Radiation Measurement (ARM) project is responsible for obtaining field measurements and developing models to better understand processes that control solar and thermal infrared radiative transfer in the atmosphere. To facilitate the easy exchange of data among researchers, field measurements are collected and transformed into a common data file format. Header information from these files is documented on ARM's Data Object Design (DOD) Web Page. The accurate representation of the file format is a valuable reference for ARM data customers, engineers and scientists. Over time, the need has developed for dynamic access to header files for the many instruments used in the ARM program. Unfortunately, because the existing web page is manually generated, it is not uncommon for there to be inconsistencies between an instrument's file format and the web page documentation. Dynamic generation of the web page using instrument data files will provide for almost real-time updates of the webpage and eliminate the possibility of user introduced errors. This paper describes the design, development and implementation of applications that automate the creation and update of files posted on the DOD web page using PERL scripts, eXtensible Markup Language (XML) and PHP. Employing dynamic access to header files improves the quality of information reported and decreases resource requirements needed to generate information, which has the added benefit of reducing project costs. ARM is committed to providing long-term, high-quality climate data to the scientific community. This work is a small portion of a much larger project developed to meet the Data Documentation requirements for updated instrument DODs of ARM datastreams as detailed in the Data Management and Documentation plan.

Automation of Training Qualification's Data Reports. GONZALO GUZMAN (University of Washington, Seattle, WA 98195) LOWELL HOWARD (Pacific Northwest National Laboratory, Richland, WA 99352).

The Training and Qualifications Department of PNNL is responsible for developing most of the web-based training for PNNL staff and visitors. Self-assessment reports, which measure the effectiveness of web-based training, are part of improving training applications. Two main reports that are created for web-based training (WBT) are a WBT effectiveness report and a cost avoidance based report. The WBT effective-

ness report measures the number of students who took a web-based training course and collects Kirkpatrick Level 1 feedback unique to the date those employees or students took the course. The cost avoidance report compares the cost of classroom delivery method of training to all other delivery methods and measures the amount of money saved by providing web-based training. These reports are very time consuming since the current method used to do these reports involves looking at the statistics for each course individually. To make this procedure more expeditious, since the current time to create a report is about a week, data collection was automated. Using a database-reporting program named Crystal Reports and some Active Server Pages, automation of the report data was accomplished during this internship. In the future the method used to automate the data in the WBT effectiveness and cost avoidance reports will be applied to all reports designed by the Training and Qualification group.

Developing a Biological Problem Solving Environment. LISA NUFFER (Utah State University, Logan, UT 84322) GEORGE CHIN, JR. (Pacific Northwest National Laboratory, Richland, WA 99352). To meet the challenges of an increasingly complex scientific landscape, biologists must be equipped with appropriate tools. Our goal is to develop an environment that allows biologists to focus on the science involved in computational experiments rather than the management of the many necessary resources and tools, and also gives them the capability to express their scientific knowledge in a form that is intuitive and natural. The product of this research is a conceptual biological problem solving environment prototype (BioPSE) that specifies a system of computational resource management and visual scientific concept modeling environment.

Developing Temperature Monitoring Software for the Temperature Investigating Mobile Automaton (TINMAN) Project. JEFFREY SCHERPELZ (Harvey Mudd College, Claremont, CA 91711) DEBK HOPKINS (Pacific Northwest National Laboratory, Richland, WA 99352).

Cooling supercomputers is an expensive task, especially when some of the cooling goes to waste. Using a system to monitor temperatures in the room and dynamically adjust the flow of cold air, it is hoped that the costs for cooling the Molecular Science Computing Facility supercomputer at Pacific Northwest National Laboratory can be reduced. We designed a system which uses a robot called TINMAN (Temperature INvestigating Mobile AutomatoN) to automatically monitor air temperatures in the room. This data is combined with data from the supercomputer, heat exchangers in the room and floor vents to compile a temperature map of the room. The floor vents are connected to the monitoring computer which can dynamically open and close louvers to adjust air-flow based on the temperature data in the room. This paper discusses the design, structure and development of the software used to coordinate the data. In addition to gathering the data, the program creates a log of data for the past week, and serves both current and old data to a graphical user interface (GUI) client that can be run on a separate computer. The GUI client can be used to monitor the temperatures in the room, and manually control the floor vents and robot. The current status of the software is reported on. Finally, future work to complete the requested functionality and other improvements are discussed.

Development of a Geographic Information System Based Dust Dispersion Modeling System for Use in the Planning and Implementation of Military Training Exercises. DUARD CRANDALL (Columbia Basin College, Pasco, WA 99301) FREDERICK C. RUTZ (Pacific Northwest National Laboratory, Richland, WA 99352).

Military maneuvers and training exercises are essential for national and world defense. These maneuvers must however be performed in a manner that will have a minimal effect on the environment and local civilians. As residential areas continue to develop near military sites, possible impacts from military traffic and exercises to these areas begin to become of greater concern. Concerns facing the military include the effects of particulate air quality and atmospheric dust dispersion caused by such maneuvers. To aid the Department of Defense with this problem, Pacific Northwest National Laboratory proposed a plan to develop, document and test a modeling system for use in dust dispersion reduction and management near government sites. To accomplish this task a user interface was developed that would be user friendly yet sophisticated enough to accommodate the needs of the client. One such need is to integrate a geographic information system (GIS) with the dust dispersion modeling software. This allows the user to enter the point, area, or line source required for the model runs. Incorporating the GIS with the software will also allow the user to view plume rise and expansion over actual data maps of the desired site. Data collected during previous field studies will be used to verify the results generated by the dust dispersion models. Thus utilizing historical, current, and

user defined data, near real-time dust dispersion models will be able to aid in estimating and minimizing the effects of military exercises on the environment and nonmilitary personnel.

Development of a Web-based Information Management System to Support the Chehalis Basin Characterization. SHERI WILES (Big Bend Community College, Moses Lake, WA 98837) LANCE W. VAIL (Pacific Northwest National Laboratory, Richland, WA 99352).

Grays Harbor County (GHC) has requested that the U.S. Army Corps of Engineers (Corps) study the feasibility of restoring fish and wildlife habitat and flood reduction in the Chehalis Basin. This requires a basin-wide environmental characterization to provide the information required to optimally allocate and schedule the resources available for restoration. Ultimately the Corps must identify, prioritize and initiate the optimal set of restoration actions. Selecting amongst the vast number of combinations of feasible actions requires a systematic and information-driven approach. Pacific Northwest National Laboratory (PNNL) has undertaken the effort to provide the information and information management system (IMS) required to clearly articulate the tradeoffs between various actions. The scope of this effort is to provide the characterization information and its associated IMS in a manner that ensures that subsequent decision-making activities are fully supported. This IMS must integrate a diverse suite of physical-process models, habitat-impact assessment models, and web-based data management and visualization tools. As part of the project to develop this IMS, a database-driven web content delivery system was developed and implemented. This provides drill-down through a continuously expanding database of content. This system is being expanded to incorporate the specific needs of distributed data and models that are used in an environmental assessment. The IMS provides an adequate metadata archive to ensure comprehensive drill-down through models and data (both local and remote). This metadata database and its associated model manager will allow a considerably increased level of automation that is expected to increase the number of alternatives that can be considered and analyzed by a factor of 100. The metadata database will also ensure the highest degree of accessibility by making enabling comprehensive drill-down through the characterization information to the stakeholders.

Documentation for ApplicationLink. KRISTY HUSTON (Columbia Basin College, Pasco, WA 99301) MARY SUE HOXIE (Pacific Northwest National Laboratory, Richland, WA 99352).

ApplicationLink is a data-driven Web application that allows faculty and college students from around the world to apply for internship programs available within the U.S. Department of Energy and its national laboratories. ApplicationLink was developed in Lotus Notes/Domino, which is an integrated software program for developing web-based applications. Because of rapid growth, the system documentation has become outdated or is nonexistent. Some substantial requirements needed to be added in the midst of development (e.g., SULI was initially supposed to be for one term and then it changed to three terms). Since the first rollout of the system in October 2001, there have been new features and functionality added and new applications added. Growth of the system has made it more difficult for developers to maintain the system. A poster designed to display the programs information onto a central location, to help with system maintenance, meta-data. Flow-charts of the application process; along with the filling out of an application through accepting an offer will accompany the information on the poster. The documentation retrieved and organized will be a valuable reference guide to programmers. ApplicationLink is committed to allowing all persons the opportunity to apply for one of the prestigious internships offered. This work is a small portion of a much larger project developed to meet the ongoing needs of people all around the world.

Error Dependency on the Courant and Peclet Numbers in Leonard TVD Solute Transport Simulations. DALE MECK (Cornell University, Ithaca, NY 14850) MARK D. WHITE (Pacific Northwest National Laboratory, Richland, WA 99352).

Practical application of numerical simulation to model subsurface solute transport is constrained by execution time. Execution time is dependent on processor speed and code architecture, but more importantly on the computational efficiency of the transport algorithm and the temporal discretization. The explicit Leonard Total Variational Diminishing (TVD) algorithm was designed to reduce the numerical dispersion often generated by other algorithms in advection dominated transport. For conservative solutes, two dimensionless parameters characterize the transport regime. The Peclet (Pe) number measures the relative contributions of dispersion and diffusion to advection and the Courant (Cr) number relates the displacement of a solute particle per time step to the spatial grid size. A two-dimensional patch source problem was modeled with the Subsurface Transport Over Multiple Phases (STOMP) simulator developed at Pacific Northwest National Laboratory and compared

with an analytical solution to determine the accuracy of the simulation for various Cr and Pe number combinations. The longitudinal and transverse dispersivity were also varied to determine whether the error dependency was problem specific. A modified relative sum of square errors method was used as a global quantitative estimate of the error associated with each simulation. Error plots indicated that the TVD transport algorithm simulation errors are strongly dependent on the Cr and Pe numbers. Simulations with Cr numbers between 0.5 and 0.6 yielded more accurate results as long as the Pe number was greater than ~20. When the Pe number was less than 20, however, the results improved as the Cr number decreased. The ratio of longitudinal to transverse dispersivity did not affect the error dependency significantly. Similar tests against analytical solutions should be conducted to determine whether the obtained relationship is consistent enough to be considered general purpose. An algorithm to automatically control the Cr number could then be incorporated into STOMP to minimize simulation errors.

Implementing Remote Sensing into Heritage College Curriculum. ANDREW DAUBIN (*Heritage College, Toppenish, WA 98948*) KAREN STEINMAUS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

This research activity was conducted at the Pacific Northwest National Laboratory (PNNL) in Sequim, WA by Andrew Daubin from May 19, 2003 to July 25, 2003. This research was sponsored by Heritage College, and co-funded under a NASA Partnerships Awards for the Integration of Research into Undergraduate Education (PAIR) Grant (NRA 02 OEOP-04) and through the Department of Energy (DOE) Science Undergraduate Laboratory Internship (SULI). The purpose of the internship was to assist in the implementation of a remote sensing program at Heritage College. During the ten week internship the following were accomplished: HTML based remote sensing tutorial, Step-by-step tutorial: Overlaying shape files on image files, Hood Canal Bridge field work, Yakima Training Center field work, and Lidar literature research.

Increasing Efficiency in Software Testing by Implementing Auto Testing. JEREMY TEMPLETON (*University of Utah, Salt Lake City, UT 84112*) GARIANN GELSTON (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The increasingly need to more efficiently test software has become evident in recent years. Not only are the software testing steps repetitive, but thousands of dollars are spent testing and documenting the changes. Auto testing is the concept of writing code to allow the computer to test certain aspects or requirements of software without human interaction. This paper describes a general format of how to write auto test code, which proved to be effective. When an auto test is executed, two documents are simultaneously produced: a test plan, which describes the steps used to test the software, and a status page, which shows whether the requirements passed or failed. The paper addresses several solutions for the challenges that arose from implementing this new form of testing. Although auto testing has proved effective for testing most aspects of software, it has limitations, which are also described. Despite these limitations, auto testing is an innovative way for scientific companies to save time and money and should be considered for testing new software.

Position Tracking of a Mobile Robot in an Unknown Environment. KEITH HERRING (*University of Illinois, Urbana-Champaign, IL 61820*) STEWART MOOREHEAD (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Localization in mobile robotics involves the estimation of a robot's pose within its environment using sensor data along with environmental knowledge. One type of localization problem, position tracking, assumes that the initial pose of the robot is known. Kalman Filtering has been found to be an optimal solution to position tracking when appropriate assumptions are made. This paper looks at how Kalman Filters can be used to handle position tracking when there is no prior knowledge of the environment. A Kalman Filter suitable for the GOAT robot has been implemented and tested with results listed.

TAC: Using Cytoscape for Visualization of Proteomics Research Results. MEGAN GRIFFITHS (*Southern Utah University, Cedar City, UT 84720*) GORDON ANDERSON (*Pacific Northwest National Laboratory, Richland, WA 99352*).

In just a few years, dramatic technological advances in biological mass spectrometry and high sensitivity separation systems have enhanced the ability to identify proteins from small quantities of cells. Cytoscape is a bioinformatics software platform for visualizing molecular interaction networks and integrating these interactions with gene expression profiles and other state data. The purpose for investigating Cytoscape was not necessarily to view interactions between proteins, but rather to see what the possibilities of graphing with Cytoscape were. Translates

Access to Cytoscape (TAC) is a software program written in Visual Basic 6 to translate data from a Microsoft Access database into a file that is readable by Cytoscape.

Using Graph Traversal Algorithms and Ontologies to Select Topic Order. MICHELLE BEGAY (*Arizona State University, Tempe, AZ 85287*) RYAN E. HOHIMER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Initially starting my participation on this ongoing project was to do extensive research. I had to research some background information about ontologies, knowledge base, and graphical user interfaces. The main programming language that I used and implemented some pseudocode with was Java. I discovered that we can use graph traversal with ontologies to automatically suggest an order of presentation of information. Eventually the scientist and their ongoing research projects will advance to higher levels of Artificial Intelligence. This research will help companies and the general public coordinate with the rapidly ever-changing technology environments.

Visualization of Well Data Supporting a Three-Dimensional Model of Groundwater and Contaminant Flow at the Hanford Site. KEITH DERAM (*Big Bend Community College, Moses Lake, WA 98837*) PAUL D. THORNE (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The plutonium production at the Hanford site in Richland, Washington has produced millions of gallons of radioactive waste. Wastes were discharged to large underground steel tanks, surface trenches, cribs, and ponds. Some of these tanks have leaked and radioactive contaminants seeped into the soil and ground water from these waste disposal practices. The purpose of this study is to display ground water radioactive contaminant flow in the subsurface sediment at the Hanford site as a 3-dimensional model. EarthVision (EV) software was used to generate 3-D images of the site geology and the subsurface contaminant plumes. Data was compiled from approximately 500 on-site wells, the geologic structure, and a surface grid of the Hanford site. Merging of these images created combinations of different geologic layers and well paths. UNIX based script code was written to sequence these geo-spatial images, displayed as iso-surface images, and viewed in 3-D animation. This technology is used to visualize where ground water and contaminants are flowing below the surface of the Hanford site. In addition to environmental applications, EV technology can be used to create and display 3-D models and visualizations of any spatially referenced data, ex: Mining Analysis, Oceanographic Investigation, and Oil and Gas Exploration.

A Flexible Data Acquisition System for Small Experiments. FRANCIS SPALDING (*Cornell University, Ithaca, NY 14850*) DORI BARNES (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

Data acquisition is an integral part of many experiments, but the development and maintenance of a data acquisition system can be a time-consuming process. Smaller experiments may not have the resources necessary to create and sustain a customized data acquisition system. This document presents a program structure for creating a flexible data acquisition system that can be shared by multiple small experiments. The example used is that of the Liquid Metal Experiment (LMX) and Magneto Rotational Instability Experiment (MRI) at the Princeton Plasma Physics Lab. The experiments share a laboratory as well as a computer with LabVIEW and data acquisition hardware and software. Both experiments plan to modify the devices used in the experiment in the near future. To accommodate both the current experiments and as many of their future iterations as possible, the LabVIEW program provides the ability to interact with a large number of data acquisition devices located in the laboratory. The user chooses a subset of these devices for use with each run and then sets the parameters for the selected devices. To facilitate the transitions between multiple configurations of devices, the program allows configurations to be saved and reloaded.

Development of Tokamak Simulation Code (TSC) Post Visualization Viewer. MIO SUZUKI (*University of California, Berkeley, Berkeley, CA 94720-1730*) ELIOT FEIBUSH (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

New visualization viewer processor for Tokamak Simulation Code (TSC) is developed. The new graphical interface is written in Fortran 90, and it processes numerical data produced by TSC takes advantage of graphical software called ElVis. Use of ElVis makes collaborative visualization efforts from multiple locations possible, and it provides greatly enhanced graphics that are apt for major publication purposes. The new post-processing program, Tscplot, reads TSC outputs as netCDF (Net Common Data Format) files and creates four types of plots: 1d plot, time-history plot, 2d-contour plot, and 3d-space-time plot. Users

would choose the plot type and generate the plot of choice by simple commands. The generated plots can be saved on the computer as post-script file, and be available for viewing by appropriate post-script viewers. To increase interactivity with users, verbosity level option is implemented in the code of Tscplot such that users are able to either add or remove extra description of the program depending on their familiarity with the TSC and TSCplot. The comparison between new and old graphical interface is summarized in a table (Table 1), from which the apparent advantage and superiority of the newly developed visualization viewer is observed.

Cosmic Ray Analysis Environment (CRAnE): A Java Analysis Studio Based Data Acquisition System for Cosmic Rays. MANUEL REYES (*Westmont College, Santa Barbara, CA 93108*) TOM GLANZMAN / WILLY LANGEVELD (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

Cosmic Ray Analysis Environment (CRAnE) is a software tool designed to collect and plot data from a cosmic ray telescope (CRT) connected to a computer serial port. As a plugin to Java Analysis Studio (JAS), CRAnE provides visual displays of incoming cosmic ray rates as they are detected. In an effort to make the program user-friendly, it operates through a graphical user interface. This paper describes the features of CRAnE and includes installation and operation instructions in the appended user's manual.

Interfacing the General Purpose Interface Bus (GPIB): The Generic Approach. SHARON CHAO (*University of California, Berkeley, Berkeley, CA 94720*) LINDA HENDRICKSON (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

With the capability of interfacing an extensive band of instruments, the General Purpose Interface Bus (GPIB) has become an integral part of computer systems. For the purpose of optimizing its universality, an interface between the user and the GPIB devices can be implemented to allow nonspecific commands to be used. In addition to writing a generic interface that can be applied in MATLAB, GPIB instruments can also be accessed through the Experimental Physics and Industrial Control System (EPICS). This option was initially explored when the EPICS support for GPIB was built, and then added to the Input Output Controller (IOC). Subsequently, hardware modules could be attached to the VME crate of the IOC, and configuration data could then be read to the database layer. This procedure, however, did not meet generality of the specifications, so the former option was investigated. When the interface was ready, the oscilloscope, arbitrary waveform generator, and various other GPIB devices were connected to the LAN-GPIB gateway for testing. This project would be useful as a diagnostic tool for several Next Linear Collider Research and Development (NLC R&D) applications such as the NLC Test Accelerator (NLCTA) and 8-pack, used to demonstrate beam acceleration; feedback on nanosecond timescales (FONT), used to demonstrate control of beam collisions; and the vibration project, used to demonstrate final focus vibration stabilization.

Designing a C++ Application that Statistically Reduces Accelerator Control System Data. VIRLIKA PRAYER (*Norfolk State University, Norfolk, VA 23504*) CHRISTOPHER LARRIEU (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

This paper discusses the development of a C++ computer program that retrieves control system data from a network server and executes statistical reduction upon the data. The archiving system stores a lot of control system data that can be difficult to deal with, therefore it is essential to provide the capability to statistically reduce it. One technique of statistically reducing data to a set of smaller statistics is called quantization. Quantization makes the information easier to understand, since the number of data points is greatly reduced. The program is efficient and maintainable. To minimize memory use, it employs Welford's Algorithm to calculate running statistics, which makes it possible to avoid storing all of the data in memory. Comments are dispersed throughout the code to increase the program's maintainability. The implementation of good software engineering skills is important when devising any computer program.

ENGINEERING

Advanced Fuel Cycle Initiative. JEREMY ROBISON (*Brigham Young University—Idaho, Rexburg, ID 83440*) WESLEY BENJAMIN (*Argonne National Laboratory, Argonne, IL 60439*).

The AFCI (Advanced Fuel Cycle Initiative) program necessitates a need for a glovebox to enable fabrication of non-fertile, actinide burning fuels, and testing of experimental fuels. We designed a glovebox with needed equipment and environment to produce two types of fuel, metal-matrix dispersion and a nitride pellet fuel. My project was to focus on the en-

gineering design process for the pressure control systems that provide an inert atmosphere inside the glovebox, as well as final equipment and shielding installation. The three pressure control systems are an integral part of the purification system allowing minor adjustments to be made to enhance glovebox operations. The primary pressure control system controls the glovebox pressure between -0.5 and -1.0 in. H₂O. Adding Argon upon reaching the low set point and exhausting argon upon reaching the high set point. The secondary system performs the same functions at the set points of -0.1 and -2.5 in. H₂O. The tertiary system is a fail safe system comprised of oil filled bubblers connected to a suspect exhaust system. The bubblers relieve at ±3.5 in. H₂O. Future work will continue until the glovebox becomes operational in July 2004.

Automobile Shredder Residue Plastics Separation by Froth Floatation. ALAINA TERZICK (*Northwestern University, Evanston, IL 60201*) BASSAM JODY (*Argonne National Laboratory, Argonne, IL 60439*).

Waste disposal facilities are becoming less useful as they accumulate copious amounts of waste. Much of this waste can be reused or recycled, including automobile parts. Cars can be stripped of functional parts, shredded, and the metals can be recycled. The metals from the car are separated from the waste, leaving automobile shredder residue (ASR). The primary objective of the ASR project is to develop and implement processes for the separation of the ASR, including the retrieval of certain recyclable plastics from the ASR material. The processes for separating these plastics include froth floatation. Froth floatation involves the separation plastics of equal densities from each other. The majority of the research performed in this lab involves determining through experimentation the ideal sets of conditions (specific gravity, surface tension, pH, etc.) to be used in order to separate the valuable plastics at high purities and yields. These plastics include polystyrene, polypropylene, polycarbonate, polyvinyl chloride, nylon, and acrylonitrile butadiene styrene (ABS).

Cathode Materials for Rechargeable Lithium Ion Batteries. LIS-TOWEL AGYARKO (*The University of Illinois at Chicago, Chicago, IL 60653*) KHALIL AMINE & ILIAS BELHAROUAK (*Argonne National Laboratory, Argonne, IL 60439*).

This paper reports on lithium iron phosphate (LiFePO₄) as a novel cathode material for rechargeable lithium ion batteries. Lithium iron phosphate was synthesized by solid-state reaction, using iron (II) oxalate, ammonium di-hydrogen phosphate and lithium carbonate as precursors. The structure of the material was characterized by X-ray diffraction and the thermal stability was investigated using thermo gravimetric analyzer (TGA) and differential scanning calorimetry (DSC). The experimental results indicate that there is no capacity fading for this olivine material and that it has an outstanding cycling capability which is not affected by high current densities. Furthermore, LiFePO₄ is thermally and structurally stable and can demonstrate a charge/discharge flat voltage of 3.4V. However, future research work must focus on the improvement of the poor electronic conductivity of the material.

Characterization and Image Correction of a Large-Area Flat Panel Cesium-Iodide X-Ray Detector. ZACHARY METZGER (*College of DuPage, Glen Ellyn, IL 60137*) WILLIAM A. ELLINGSON (*Argonne National Laboratory, Argonne, IL 60439*).

Large-area direct read-out flat-panel detector systems represent the most recent development in digital X-ray imaging. The purpose of this study is to characterize the newly instituted amorphous silicon detector and determine a more effective pixel correction technique. An X-ray detector's capabilities are typically defined through its performance under various controlled conditions such as current levels, object size, detail size and object density. From acquired images, edge-response functions, line-spread functions, and modulations transfer functions, which are all indicative of a detector's precision, can be derived and compared to industry standards. A pixel correction method based on Lambert's law of absorption is instituted to create a uniform pixel response and filter errors.

Coiling Coil Performance Study. ISAIAH ABRAMSON (*Hebrew Theological College, Skokie, IL 60077*) MARVIN KIRSHENBAUM (*Argonne National Laboratory, Argonne, IL 60439*).

The Advanced Photon Source is cooled using a chilled water closed loop system. It consists of a series of chillers located in a central plant and a series of Air Handling Units located at different points around the campus. During the intermediate weather days the chilled water is not returning to the chillers at a high enough temperature, sometimes causing the chillers to shut down or the supply water temperature set to become elevated. A series of experiments were conducted, modulating the different variables such as valve position, mixed air temperature, chilled water temperature, and fan position. The results show that little can be done to fix the problem through a change in the controls sequence. One

possible solution is to divert some of the return water into the supply water line or through the preliminary heating coil. This initial portion of research is part of a larger project to optimize the cooling system.

Database Management and Document Control. DOUGLAS CAGNEY (Purdue University, West Lafayette, IN 47906) KYUNG (PAUL) CHOI (Argonne National Laboratory, Argonne, IL 60439).

Database Management and Document Control are organizational requirements in any business. Properly storing current information is the way to safeguard against miscommunication between a design team and a production team. Up-to-date paper copies of documents (in this case CAD drawings) must be kept for reference purposes while electronic copies must be kept for making any necessary revisions to an existing design. Every time a drawing is updated and released, it gets released as the same drawing number, but as a different version. Paper copies are maintained by a group called the Document Control Center (DCC) while electronic copies are held in a file called EDS Share. I needed to make sure that the most recent drawing versions that existed in both drawing locations (the DCC and the EDS Share file) matched. If there was a discrepancy between versions, I was to take the latest version and update it to the other location. This was done for an entire Insertion Device (ID) assembly set located on the Advance Proton Source (APS) ring. I also had a concurrent project that involved releasing a set of new drawings on the Linear Accelerator (LINAC) to the DCC and electronically organizing them in an inter-office database management system called Pro-Intralink.

Design of Upgrade for Beam Emergency Shut Off Current Monitor. LAV ROHATGI (State University of New York, Stony Brook, Stony Brook, NY 11794) OM SINGH (Argonne National Laboratory, Argonne, IL 60439).

The Beam Emergency Shut Off Current Monitor (BESOCM) is a part of personnel protection system, which has been implemented in the Advanced Photon Source to prevent the accidental injury of people due to machine or operational failure, i.e. it is designed to prevent the unintentional acceleration of high beam currents that could result in unexpected and hazardous radiation fields. Though the BESOCM, which was first implemented in 1993, has proved to be an exceptionally reliable system, time has come to modify and upgrade it in the light of new technology to make it even more efficient and reliable. BESOCM is designed to be a standalone device and thus it is not linked with the main system. However it has provision to be connected online so that it can provide a real time status of the system to the operator in the control room. The next phase of upgrade also envisages to implement this system by connecting the inputs to a PLC and designing the EDM screens and writing the code for the driver to link the inputs to the system so that in case of failure of the beam and the triggering of BESOCM, the operator would know exactly what was the cause of the alarm, without leaving the control room.

Effects of Laser Surface Micro Texturing on Friction. RAE DINS-MORE (University of Alaska Fairbanks, Fairbanks, AK 99709) OY-ELAYO AJAYI (Argonne National Laboratory, Argonne, IL 60439). Power losses due to friction are usually over a small physical area, however there are so many of them in vehicles and industry that if friction can be significantly reduced, it would result in enormous financial savings. Tests done to date indicate that a series of pores (dimples) burned into the surface with a laser can reduce friction; however the constraints are not clear. The testing undertaken was to clarify exactly under what load, or speed friction is reduced, so the test variables were load and speed. There were four combinations of dimpled and undimpled samples, three different loads (5, 10 and 20), and eight different speeds (in rpm which is increased and decreased so that is fifteen segments). This gave twelve (forty five minute) tests in all. The steel samples are: HC 13 steel for the flats, SS 300 steel for the rollers. Due to personal health and technical challenges, not enough testing has been completed to draw clear conclusions. However it is clear that surface texture does impact friction, and the preliminary results indicate that at larger loads a undimpled flat and a dimpled roller give the lowest coefficients of friction.

Evaluation of Materials for Advanced Nuclear Reactors. KENT WARDLE (Brigham Young University, Provo, UT 84602) JAMES I. COLE (Argonne National Laboratory, Argonne, IL 60439). This study is the initial phase of an overall project focused on identifying and evaluating materials for GenIV reactor designs with particular focus on the SCWR. The focus of this initial phase was the characterization and analysis of the microstructures and grain sizes of T122, MA957, 800H, and MA754 alloys preliminary to further evaluation and irradiation testing. We verified the duplex nature of the ferritic-martensitic T122 steel identifying the martensite matrix and ferrite stringers. In concord

with previous studies the MA957 alloy had very thin grains elongated in the extrusion direction. TEM analysis identified the presence of the nanometer-sized yttria oxide particles. Alloy 800H had a very large grain structure that also exhibited annealing twins. Optical and SEM analysis of alloy MA754 showed the presence of three phases each with a uniform dispersion of yttria oxide. The results of this study will be employed as a base-line for future irradiation testing and evaluation to determine adequate materials for advanced reactor components.

Hydrolysis of Silicalite-Supported Magnesium Chloride. BRENDAN BOYLE (University of Pennsylvania, Philadelphia, PA 19104) MICHAEL SIMPSON (Argonne National Laboratory, Argonne, IL 60439).

Hydrolysis of Magnesium Chloride is the first step in a thermo-chemical/electro-chemical process involving the Reverse Deacon reactions and the electrolysis of hydrochloric acid. $(1) \text{MgCl}_2(\text{s}) + \text{H}_2\text{O}(\text{v}) \xrightarrow{-500\text{C}} \text{MgO}(\text{s}) + 2\text{HCl}(\text{g})$ $(2) \text{MgO}(\text{s}) + \text{Cl}_2(\text{g}) \xrightarrow{-400\text{C}} \text{MgCl}_2(\text{s}) + \frac{1}{2}\text{O}_2(\text{g})$ $(3) 2\text{HCl} \text{-(e}^-\text{)} \rightarrow \text{H}_2(\text{g}) + \text{Cl}_2(\text{g})$ Net Rxn: $\text{H}_2\text{O}(\text{v}) \rightarrow \text{H}_2(\text{g}) + \frac{1}{2}\text{O}_2(\text{g})$ The successful running of the hydrolysis reaction being of obvious importance to the entire process, my work focused on making it easily scaled to an industrial size. This was done by loading MgCl_2 powder into a powdered silicalite, a low-aluminum ZSM-5 type zeolite. Once in silicalite, the magnesium chloride molecules should be well spaced and separated, allowing for enhanced kinetics and eliminating the degradation of the salt crystal that occurs when hydrolyzing larger MgCl_2 particles. Loading salt into the silicalite was accomplished by heat-induced occlusion and quantified by free chloride tests on solutions made from salt/silicalite mixtures. Though repeatability was poor, enough excellent results were seen to merit further research and fine tuning of the procedure. Occluded samples of various percent-loadings were hydrolyzed by passing steam over them in a 500°C quartz tube furnace reactor. All steam and evolved HCl went into a titration cell, where a known volume of 0.102 N NaOH solution was titrated against the acid. Volume NaOH titrated was recorded over time to give a hydrolysis reaction rate curve. These curves were then compared to those obtained from hydrolysis of powdered MgCl_2 . Comparison of the hydrolysis curves show that MgCl_2 in silicalite is reactive towards hydrolysis, though the extent of reaction varied and was not always comparable to powdered MgCl_2 . Stability of silicalite in this process is imperative, as an industrial scale-up of the process will require a zeolite support that maintains its integrity throughout. To get a grasp on the stability of silicalite from drying to hydrolysis, we used X-ray powder diffraction. A dry silicalite baseline was first obtained and found to be in excellent agreement with XRD database patterns. Patterns for loaded silicalite and then subsequently hydrolyzed silicalite were taken and compared to the baseline. No peak shifts or meaningful changes in intensity were observed for any series of samples run, giving us an excellent indication that our silicalite is not breaking down or degrading at any stage of the process.

Potential of Hydropower to Supply More Power in the United States. DANIEL FEINAUER (BYU - Idaho, Rexburg, ID 83460) CHARLES SOLBRIG (Argonne National Laboratory, Argonne, IL 60439).

This report is an evaluation of hydropower. The report describes hydropower as electricity produced by hydropower. The report is focused on dams and their production of hydropower. Four main types of dams are discussed. Arch dams are dams shaped like an arch using its arch to support the reservoir. Gravity dams are very thick and heavy usually made out of concrete; they use their weight to support the water in their reservoir. Buttress dams are dams that use buttresses to support the reservoir and dam. An example of a buttress dam is a multiple arch dam. Embankment dams are like gravity dams, but are made of earth or rock. The four main types of turbines; Pelton, Francis, Kaplan, and Banki are briefly described. The pros and cons of hydropower are discussed. A look at the safety of dams and a list of significant dam failures are provided to inform the reader on the possible dangers of dams and their safety. The reader will also discover in brief the possible damages done by dam construction. A table of some significant hydropower plants and the surface acres of their reservoirs are provided to show the reader roughly how much land is flooded to produce hydropower. The reader also will be informed on the average cost to produce and operate hydropower. The main purpose of this report is to help the reader make an educated stand on whether they should be for or against hydropower. The possible future expansion of hydropower is discussed. The results of previous studies of hydropower are discussed to determine the amount of hydropower that can be used in the US. Obstacles that must be overcome for hydropower to reach its maximum potential are provided. This report should give the reader a basic knowledge of hydropower's role in the energy picture.

Spectroradiometer Calibration, Comparison, and Performance.

DANIEL STEEVER (University of Colorado, Boulder, Co 80301)
DARYL MYERS (National Renewable Energy Laboratory, Golden, CO 89401).

Spectroradiometric measurements are key to quantifying the performance of spectrally sensitive photovoltaic (PV) devices. This project is an evaluation of the National Renewable Energy Laboratory's spectroradiometry systems. We identify sources of, and quantify measurement uncertainties among three spectroradiometers and make recommendations for improvement. Two spectroradiometers we tested (OL 750 and OL 754) were calibrated at temperatures between 20°C and 22°C. The third spectroradiometer tested, an LI-1800, was calibrated with a temperature-controlled detector at 20°C. All three spectroradiometers have an expected wavelength dependent measurement uncertainty ranging from ±1% to ±4%. We tested the three spectroradiometers outdoors by making simultaneous solar irradiance measurements over a temperature range of 13.5°C to 24.7°C. We measured global horizontal, 40° tilt, global normal, and direct normal spectra. We analyzed the irradiance data for deviations between instruments exceeding the expected uncertainty limits. Deviations between the LI-1800 and the OL units were greater than ±2% in the 450-650 nm range. Irradiance differences increase with an increase in ambient and detector temperatures. We tested the LI-1800 performance with a commercial and a custom temperature control system using an environmental chamber and stable light source. Without auxiliary water-cooling, thermal run-away occurred at 38°C. With the custom temperature controller, data at wavelengths below 1000 nm were within the range of expected variation, but data at wavelengths above 1000 nm were not.

Locating and Identifying Electrical Power Poles Using Geographic Information System.

ANDREW MIKLOS (College of DuPage, Glenn Ellyn, IL 60137-6599) **RONALD RICHARDSON** (Argonne National Laboratory, Argonne, IL 60439).

The project's goal was for the Plant Facilities and Services Division (PFS) to update the utility drawings to include the electrical power pole numbers. The current utility drawings used by the electrical maintenance personnel were created in the 1970's and are out of date. PFS coordinated with the Environmental Assessment Division (EAD) to achieve this task. EAD obtained an aerial photograph of Argonne National Laboratory and manipulated it using Geographic Information Systems (GIS). With GIS, EAD was able to locate all the poles and color them to stand out from the rest of the photograph. Each pole was assigned an arbitrary number and matched with its coordinates on the Argonne grid. The GIS was put onto a pocket PC to be used by PFS. Each pole in GIS could be matched with the poles on the old utility drawings. By clicking on each pole, an attribute popped up displaying the arbitrary number, coordinates, and a blank field where the actual number was inputted. Some fieldwork was required for verification. Once all the numbers were checked, the GIS data was transferred into a Microsoft Excel spreadsheet where additional comments were inputted, such as if the pole had a light on it. Finally, the GIS coordinates were converted to the coordinates used in AutoCAD to produce an updated utility drawing. Now, the linemen can use the AutoCAD drawing to view the pole locations and numbers. In the future, anyone could update the GIS information and synchronize it with the AutoCAD utility drawing.

Mobile Melt and Dilute Process.

WILLIAM SKERJANC (Idaho State University, Pocatello, ID 83201) **ERIC HOWDEN** (Argonne National Laboratory, Argonne, IL 60439).

Highly enriched uranium (HEU) is currently being stored at research reactor facilities in Former Soviet Union countries. These fuel assemblies containing HEU are a proliferation concern and a terrorist threat. There is not sufficient security in the FSU to protect this weapons grade material. The Mobile Melt and Dilute (MMD) process offers an economical solution to secure the HEU and turn it into a low enriched uranium (LEU) ingot that is less than 20% isotopic content. Depleted uranium and aluminum are added to the highly enriched fuel assemblies and melted together to form an LEU alloy ingot. The LEU ingot can later be reprocessed for other nuclear applications. The welding station design studied had to be compact, durable, and produce a weld that would pass ASME pressure vessel codes. It was determined to use an automatic welder that would sit on top of the fuel canister to secure the canister lid prior to melting the highly enriched fuel assemblies and depleted uranium and aluminum. This option meets all of the functional design requirements for the MMD process. It should be noted, however, that the MMD process and technology are still in conceptual design at Argonne National Laboratory West and Savannah River Technology Center. The welder design, as well as the functional requirements, might change as the project moves into the next stages of development.

Nuclear Engineering Economics.

KIMBERLY GAMBONE (Oregon State University, Corvallis, OR 97330) **ERIC HOWDEN** (Argonne National Laboratory, Argonne, IL 60439).

Costs for experimental projects are researched before a project is put into full action. Project coordinators research how much processes cost to operate and to repair. Because new experimental cost can not be known with one hundred percent accuracy, data is collected from similar past experiments and occurrences for comparison. Because the cost of transporting hydrogen can not be completely accurate until it has been done, estimations of the cost are made using data collected from transporting natural gas. Modeling is often a key tool in collecting reasonable data for the unknown. It is a tool used to make estimates for the cost of operation for fuel cycles. Again while not completely accurate, it helps to provide very good estimates figures. Often times funding runs short and alternate funding sources must be obtained. Organizations exist whose goals are to fund and promote research that offers the promise to improve quality of life for people all over the world. Knowing where and how to contact these organizations could prove frustrating, however; a new collection of information about such organizations in one central location eliminates such frustration.

Optimization for Lithium Ion Batteries.

XIAOQING QIAN (Washington University, St. Louis, MO 63105) **CHRISTOPHER JOHNSON** (Argonne National Laboratory, Argonne, IL 60439).

The standard, undoped spinel oxide $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and its multi-doped derivatives 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/ $\text{Li}(X \text{ Ni Mn})_2\text{O}_4$ between the voltage limits 3.5 to 5.0 V for optimization. Undoped spinel oxides were coated with ZrO_2 and CdS colloid to decrease the irreversible capacity by lessening the volatility of the cathode surface. Results suggest that these strategies may be useful in engineering new batteries to operate at 5 V in a Li cell.

Separation of Automobile Shredder Residue plastics by Froth Flotation.

TOM HILLEMEIER HILLEMEIER (Washington University, St. Louis, MO 63130) **BASSAM JODY** (Argonne National Laboratory, Argonne, IL 60439).

Recycling the resources used in automobiles will become more and more important in the future as civilization continues to use up natural resources. In order to recycle car parts, the cars must first be shredded up into a mixture called automobile shredder residue (ASR). Then the metals are separated for reuse. The residual material, commonly known as ASR is then taken to a landfill. The objective of this project is to develop processes to separate the individual plastics from ASR for recycling. The process for separating the plastics is called froth flotation. It separates ASR into its separate components by the use of a series of stages. Each stage will separate a certain material from the mixture. The main research done in our lab concentrated on finding the ideal chemical conditions to separate a variety of plastics including urethanes, polystyrenes, polypropylenes, polyethylenes, and nylons from our target plastic, acrylonitrile butadiene styrene (ABS). The chemical conditions explored were the solution density, pH, and surface tension. Future work will consist of obtaining the correct solution conditions to separate these other plastics from ASR, and then implementing these conditions in the Froth Flotation apparatus itself.

Testing of a 50% Hydrogen-50% Compressed Natural Gas (CNG) Ford F-150 Pick-Up Truck in Argonne's Advanced Powertrain Research Facility (APRF) 4WD Test Cell.

TOBYN VANVEGHTEN (University of Missouri-Rolla, Rolla, MO 65401) **DAVE SHIMCOSKI** (Argonne National Laboratory, Argonne, IL 60439).

As technologies improve, vehicles are getting more efficient and the exhaust emissions are being reduced. As emissions get even lower, more precise and accurate equipment is needed to measure the emissions of these newer vehicles. For this reason, the Advanced Powertrain Research Facility at Argonne National Laboratory was designed to test many different vehicles and is accurate and precise enough for the most advanced low emissions vehicles. A variety of vehicles have already been tested at this facility, and in this report, the test results of a Ford F-150 are presented. This F-150 has been modified to run 50% hydrogen blend. Data from an earlier test with a Ford Explorer running a conventional V6 gasoline engine was used for comparison, although the engines of the two vehicles are different sizes. In general, the F-150's emissions were close to that of the Explorer, especially for the highway cycles. The F-150 had lower carbon dioxide content in both highway and UDDS cycles and lower nitrogen oxide content in the highway cycle than the Explorer.

Three-Dimensional X-ray Computed Tomography Image Analysis Techniques. ERIC WARREN (Southern Illinois University-Carbondale, Carbondale, IL 62466) WILLIAM ELLINGSON (Argonne National Laboratory, Argonne, IL 60439).

Improvements in digital X-ray detectors and computed tomography (CT) techniques have created a need for new flaw detection and display technology. As both data acquisition and processing times are reduced and flaw detection resolution improves, the amount of data dramatically increases. However, the technology still requires a highly trained professional to analyze the resulting images. To reduce the analysis time of three-dimensional X-ray CT data sets, virtual "slicing" and "peeling" of volume data will allow once-unknown internal defects in objects to be discerned and quantified with greater efficiency.

Use of Inert Metal Anodes in Aluminum Production. LAURA STUD-NICKA (University of Dayton, Dayton, OH 45401) GREG KRUMDICK (Argonne National Laboratory, Argonne, IL 60439).

The current process to obtain aluminum metal is the Hall- Heroult electrolysis process that converts alumina to aluminum metal. The Hall- Heroult process has several drawbacks; namely energy consumption, and release of environmentally harmful gasses. This project is dedicated to finding an inert metal anode that can replace the carbon anodes that will not only lower energy consumption, but also catalyze produce oxygen instead of harmful gasses. In addition, we hope to find an anode that can last longer and be changed less frequently which will reduce labor and also the possibility of injury in the aluminum making process. Many alloys have been and are being tested using a small, 10 amp cell for 24 hours. The aluminum produced from these tests has then been analyzed for impurities of K, Fe, Ni, and Cu using Atomic Absorption Spectrometry. Promising alloys have then been tested using a 100 amp cell for 100 hours, however none of the alloys tested thus far have lasted the full 100 hours. Alloys will continue being tested and the cell design will continue being updated. Once a suitable alloy is found, it will be tested using a pilot plant.

Electronic Packaging Upgrade of a Collider-Accelerator Personnel Radiation Monitor. VIR ANGELO LONTOC (Essex County College, Newark, NJ 07102) VINCENT CASTILLO (Brookhaven National Laboratory, Upton, NY 11973).

Radiation monitoring is critical in the operation of research facilities such as the Relativistic Heavy Ion Collider at Brookhaven National Laboratory. The radiation area monitors commonly referred to as 'chipmunks' that are currently in use were designed more than two decades ago. Since then, the electronics industry has evolved. More efficient components have rendered certain components to be obsolete and unavailable on the market. This has led to the project of upgrading the chipmunk. The current effort is primarily concerned with replacing obsolete components and improving circuit designs while maintaining the existing functionality of the chipmunk. By researching different components and repackaging the chipmunk with current technology, a prototype model is being developed. The prototype displayed the same activity as that of a regular chipmunk.

Mechanical Design Study of a Superconducting Undulator. NICHOLAS LYNCH (Lehigh University, Bethlehem, PA 18015) JOHN SKARITKA (Brookhaven National Laboratory, Upton, NY 11973).

The growing experimental needs of the light source user community has led to a strong push for the development of the next generation of insertion devices, the Superconducting Undulator (SCU). The SCU will be able to produce X-rays up to three times brighter than the existing technology. The goal of this study is to develop a conceptual mechanical design that will sufficiently cool NbTi wound magnets to 4.2K, within its superconducting region, and sufficiently protect these superconducting magnets from any and all heat inputs. The recent advancements in Pulse Tube cryocooler technology provides a viable option to establish a stable coldmass while a simple thermal analysis can identify the radiation and conductive heat leaks. The use of a series of heat shields and multi-layer aluminized mylar 'super-insulation' will intercept radiation heat leaks while proper support design and material selection will minimize the conductive heat leaks. Future plans include a more complete study into other potential heat sources and an in depth finite element analysis to develop a comprehensive thermal model of the system. The results from this study are to be used in the future design and construction of a working SCU prototype to be installed within the X-ray ring at the National Synchrotron Light Source, at Brookhaven National Laboratory (Upton, NY).

Pursuing the Prototype of a New Generation of Radiation Area Monitors. MWESIGWA MUSISI-NKAMBWE (Monroe Community College, Rochester, NY 14623) VINCENT J. CASTILLO (Brookhaven National Laboratory, Upton, NY 11973).

Radiation monitoring is critical in the operation of research facilities such as the Relativistic Heavy Ion Collider at Brookhaven National Laboratory. The radiation area monitor commonly referred to as the 'chipmunk' that are currently in use were designed more than two decades ago. Since then, the electronics industry has evolved. More efficient components have rendered certain components to be obsolete and unavailable on the market. This has led to the project of upgrading the chipmunk. The current effort is primarily concerned with replacing obsolete components and improving circuit designs while maintaining the existing functionality of the chipmunk. By researching different components and repackaging the chipmunk with current technology, a prototype model is being developed. The prototype displayed the same activity as that of a regular chipmunk.

Radio Frequency Cavities in the AGS-Booster: First Fault Detecting Program. BRIGITTE HSEUH (Johns Hopkins University, Baltimore, MD 21218) ALEX ZALTSMAN (Brookhaven National Laboratory, Upton, NY 11973).

A major accelerator in Brookhaven's Collider-Accelerator Department's complex is the Booster synchrotron. It receives lower-energy particles, such as protons, from the LINAC and all sorts of ions ranging from deuterium to gold from the Tandem van de Graaft, and accelerates them to higher energy levels, before sending them into the AGS ring for further acceleration [1]. Within the Booster are four radio frequency accelerating cavities, referred to as A6, E6, A3 and B3. These cavities create electromagnetic waves of ever-changing frequencies to accommodate the perpetually increasing energy of the particles as they flow through the Booster ring. The power amplifier of each cavity consists of several components, among them a tube and power supplies. Within these components exists the possibility of certain faults occurring, each of which must be monitored and logged. The RSLogix5 software utilizes a ladder logic code to interact with a PLC that controls and monitors the cavities. The PLC has been programmed to detect a number of fault conditions and record the time and date in which they occur. Using the RSView32 software, it is feasible and advantageous to create a graphical interface for the user to interact with this fault-detecting software.

Sonochemical Synthesis of Nanophase Molybdenum-based Catalysts for Hydrodesulfurization of Transportation Fuels. ARIEL MALMQUIST (University of Idaho, Moscow, ID 83843) DEVINDER MAHAJAN (Brookhaven National Laboratory, Upton, NY 11973).

The removal of sulfur from transportation fuels is of growing concern and the introduction of nano-sized materials has proven to enhance activity of the molybdenum-based catalyst used in the hydrodesulfurization (HDS) process. The sonochemical synthesis of heterogeneous, bimetallic, Mo-based catalysts was successful in producing highly active, nano-sized particles in quantitative yields. The well-defined molybdenum hexacarbonyl ($\text{Mo}(\text{CO})_6$) and dicobalt octacarbonyl ($\text{Co}_2(\text{CO})_8$) compounds underwent sonolysis in the presence of sulfur and gamma-alumina ($\text{g-Al}_2\text{O}_3$) for a period of about 24 hours at 55°C. The resulting black slurry was purified and dried to produce a fine powder to be used as the HDS catalyst. The Transmission Electron Microscopy (TEM) micrographs showed small particles of MoS_2 on the order of 2-5 nm and larger crystalline structures of CoS of ~50 nm. X-Ray Diffraction (XRD) data displayed the characteristic nanophase MoS_2 peak and a crystalline structure pattern, but the CoS characteristic peak was distorted. Structural analyses revealed the addition of the Co-promoter changed particle geometry in the nanophase and the Al_2O_3 support reduced agglomeration and increased active site dispersion and availability, both of which, along with nano-scaling the particles, have proven to enhance catalytic activity in the HDS evaluation.

Characterization of Hazardous Materials Contained in the Test Trains Housed in the Materials Test Reactor Canal. BRIAN HANSEN (Utah State University, Logan, UT 84321) JOHN LAYMAN (Idaho National Engineering & Environmental Laboratory, Idaho Falls, ID 83415).

About 20 years ago, the United States government funded research aimed at understanding what are the causes and effects of a nuclear meltdown. This research involved sophisticated experiments called test trains, which were used in nuclear reactors to measure various parameters such as pressure and temperature during simulated nuclear accidents. Many of these test trains were stored underwater in the MTR canal, which lies just below the original reactor, where they remain today. As part of the Idaho Completion Project, the government has mandated the Decommission, Decontamination, and Deactivation of this nuclear waste. The issue of nuclear waste disposal is complicated by the presence of heavy metals and other hazardous materials. If these materials exceed regulatory limits, the waste must be buried as mixed waste. For this reason, the test trains needed to be analyzed for the type and quantity of such hazardous materials. An estimate of this nature was accomplished by studying the original test train drawings,

and by developing a model to approximate the mass of hazardous materials.

Full-Scale Structural Testing of a Double-Wide Manufactured Home. ANTHONY CRAWFORD (Idaho State University, Pocatello, ID 83209) WILLIAM RICHINS (Idaho National Engineering & Environmental Laboratory, Idaho Falls, ID 83415).

Manufactured homes house millions of families across the United States. The scope of this project is to enhance the durability, protective performance, and energy efficiency of such homes while experiencing harsh weather conditions analogous to those of tornados, hurricanes and other high wind systems. The project intends to achieve these results by examining the effects that the high winds of Arlington, Wyoming have on a (60' X 26'-8") double-wide manufactured home. A static air bag test is also to be administered on the home to produce data for various applied pressures. Approximately 190 measurement devices will monitor the movement of the home, with the data being recorded into a computer system. These devices included load cells, LVDT's, pressure taps, and displacement transducers installed throughout the home. Each device is assigned its own channel number and multiplex number and the collected data is then recorded into an Excel database where it can be broken down and correlations can be found between applied structural loads and the reactions of the home. It is hoped that the data collected will produce conclusive evidence of the areas that need attention in order for project's sponsor, HUD, to enhance the quality of manufactured housing.

Automated Generation of Superconducting Magnet Parts Using Pro/Engineer Computer Aided Design Software. THOMAS MARTIN (California State University Maritime, Vallejo, CA 94590) RAY HAFALIA (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

The Superconducting Magnet Group, of Lawrence Berkeley National Laboratory, designs and tests magnets for particle accelerators. Interactive Region Quadrupole magnets (which are used to focus particle beams) have a complex magnetic coil winding geometry that requires the use of many solid spacers to fill gaps between sets of coil winding cables. These spacers are critical support structures that constrain coil windings while the magnet is active. Because there are many spacers and several iterations that a magnet design may go through, an effort has been made to automate the design process of these coil spacers. To that end, a macro has been created in Pro/Engineer that references imported coil geometry to create and merge surfaces and then creates solid spacer parts. Currently, we can generate the coil automatically, and the spacers that fit into the coil. Work is continuing with C++ in Pro/Toolkit to modify the Pro/Engineer software to allow these two separate processes to be merged without any user interaction. It is estimated that automation of these processes will save 15 - 20 % of overall magnet development time.

Comparison of Air Handlers for Residential HVAC Applications. MICHAEL MINGEE (Virginia Commonwealth University, Richmond, VA 23223) DOUGLAS BRENNER (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

In continuing the development of energy efficiency standards, consideration has turned to air handlers (fans, blowers) used for heating and air conditioning of consumer residences. General Electric (GE) designed a prototype and sent it to the Energy Performance of Buildings Group at Lawrence Berkeley National Lab for testing. The prototype GE air handler and a production fan typical of the current market were tested in a full-scale 'house' specifically designed for testing heating, ventilation, and air conditioning systems. Tests compared efficiency and total airflow through the fan, how each reacted to restrictions in airflow, and how each fan reacted to being in a smaller cabinet. To test for a smaller cabinet, sheets of rigid polystyrene foam were placed between the fan and the cabinet walls to reduce the space between the cabinet and the fan inlet. The production fan was tested at constant speed set by jumpers on the control board. On the other hand, the GE fan was tested at constant torque, set through its computer interface. To test for a smaller cabinet, sheets of rigid polystyrene foam were placed between the fan and the cabinet walls to reduce the space between the cabinet and the fan inlet. Under the same flow restrictions (four of ten vents closed), the fans had the following characteristics: in the typical cabinet, the PSC moved 1.9 CFM/Watt at 1030 CFM and 12% efficiency, and the ECM moved 3.6 CFM/Watt at 950 CFM and 21% efficiency. In the small cabinet the PSC moved 1.8 CFM/Watt at 920 CFM and 8.2% efficiency, and the ECM moved 2.7 CFM/Watt at 740 CFM and 7.6% efficiency. At the same flow rate of 950 CFM the ECM was 37% more efficient than the PSC, at 21% and 14% respectively. On average, the ECM was 46% more efficient than the PSC. The smaller cabinet had a more drastic effect on the reducing the average efficiency the ECM than the PSC. It cut the average efficiency of the ECM by 55% and by 27% for the PSC.

Development of a High-Voltage Arc Detector for Klystron Amplifier. MARIANO RUIZ (University of Texas at Brownsville, Brownsville, TX 78523) ROGER DWINELL (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

The 88-Inch Cyclotron at LBNL is a particle accelerator in which a magnetic field causes particles to orbit, and an oscillating electric field accelerates these ions. One source of particles is the Venus Ion Source. The Venus Ion Source uses RF (Radio Frequency) to generate plasma, and also transfers energy to the plasma electrons. The electrons spiral in synchronization with a microwave frequency. This 2 kW of RF power is provided by an electron tube that amplifies electromagnetic radiation in the microwave region called Klystron amplifier. Several faults can occur to these amplifiers. Waveguides improperly terminated or changes on the plasma load create reflective power. This power is capable of damaging the amplifier. The purpose of this investigation was to design a circuit with fast response time used to detect arcs inside the waveguides and have the amplifier output automatically tuned off. The arc is visible (400-700 nm). To simulate the reflective power, an LED ($I=625$) was placed inside a waveguide. This signal was transported to the circuitry using fiber optic cabling. Several photodiodes, phototransistors, photodarlington, and Op-Amps combinations were tested for response time. The circuit was designed using a photodiode connected in photo-voltaic mode to an Op-Amp cascaded to another Op-Amp operating as Non-Inverting amplifier. The rise time of this circuit (10%-90%) is 6.05 mS and stable. The response time of the circuitry is based on adequate simple circuit design, component selection, and shielding.

Effects of Duct Leakage on Cooling Coil Loads and Fan Power Consumption. SKYLAR COX (Utah State University, Logan, UT 84321) NANCE MATSON (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

Heating ventilating and air conditioning (HVAC) systems in California commercial buildings consume approximately one quarter of the electrical energy used by these buildings and account for about half of their peak electrical requirements. The purpose of this study is to determine the influence duct leakage has on the effective coil load and the system fan power consumption. The data that was analyzed in this study was collected by LBNL's Energy Performance of Buildings (EPB) group for the "Thermal Distribution Systems in Commercial Buildings" (TDSCB) project. Calibrated leaks were installed in the ducts of one floor of a large commercial office building in Sacramento. Sensors, positioned before and after the coils on two floors (study and control) of the commercial building, took temperature and relative humidity measurements every minute throughout the nine-month testing period. Watt transducers measured fan power and flow grid pressure transducers were used to measure airflow. The thermal data was processed and utilized to calculate the cooling coil loads on a minute-by-minute basis. A weather-based normalization process was used to compare the various leakage cases (no leak, upstream, downstream, and upstream & downstream of the variable air volume (VAV) boxes). Depending on the leakage case, the coil loads and fan power consumption of the study floor were about 15%-30% larger than those of the control floor which had no modifications to the HVAC system. The most significant finding of this study is that duct leakage makes a substantial contribution to the effective coil load and fan power consumption.

Energy-Efficient Portable Luminaires for Multi-Directional Office Task Lighting. ROBERT LOVE (Tennessee State University, Nashville, TN 37209) ENGDU WORKNEH (Santa Monica College, Santa Monica, CA 90405) MICHAEL SIMINOVITCH (Lawrence Berkeley National Laboratory, Berkley, CA 94720).

Developing energy-efficient luminaires is one of the best ways to reduce energy consumption around work stations without sacrificing the productivity of the worker. The Environmental Energy and Technologies Division of Lawrence Berkeley National Laboratory was responsible for the development of portable luminaires for use in office task lighting. The designs developed for these luminaires are intended to provide more flexibility for office lighting through user operated controls. This flexibility includes features such as multi-directional lighting. High efficiency luminaires and lamps were used in the design to reduce energy cost by at least 30 percent in office spaces, while still providing an adequate level of illuminance for different tasks. A small metal grid was used as a means to easily mount the designs, and small strips of highly reflective metal were used to help build the prototype. The project took on the approach of developing designs from the outside in, to increase the chances of 100 percent market penetration. From this method designs were developed and analyzed both photometrically and aesthetically. To develop the most efficient system, complex geometrical analysis was performed to optimize lighting angles, and the dimensions of the luminaire. The final prototype consisted of two metal flaps rotating on opposite sides of the bulb. They were able to project light upward, downward, and both directions simultaneously. The flaps

consisted of highly reflective white paint, that dispersed light more evenly than normal specular material. This design was able to achieve a high illuminance for upward lighting, as well as a sufficient amount of light for downward task lighting.

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 modeling is a good way to predict the seismic response of buildings. It can help to determine the natural frequencies and the magnitude and distribution of stress throughout the building. This is the continuation of last year's research, which had built a finite-element model of the Berkeley Town House, and performed modal and spectrum analyses of the building using a finite-element computer program called ANSYS. Transient analysis is preformed using last year's model. In addition, nine modifications were made to the original building model to see how the modifications to the building affect the stress distribution. The time-history acceleration data from the El Centro Earthquake in 1940 were used as the acceleration load for the transient analysis. A command script file containing the commands for ANSYS to perform the analysis and the acceleration data was written. The results show that the maximum stress of the original model is about 12000 psi and is located at the northeast side of the building. The modified models show that the stress of the building will increase significantly if some of the structures in the basement of the building are removed. Removing structures in the basement of the building also affects the fundamental frequencies of the building. In the future, a network of wireless sensors will be installed to the building in order to compare the model with the measured data.

Finite Element Modeling: Dynamic Building Response to Seismic Loads. *Analysis of a Nine-story Berkeley Townhouse. JOHN GLOVER (Evergreen Valley College, San Jose, CA 95135) DEBORAH HOPKINS (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

Lawrence Berkeley National Laboratory's Engineering Division is developing a network of wireless vibration sensors in collaboration with Hewlett-Packard and the City of Berkeley. These sensors could be instrumental in the calculation of building responses to seismic activities as well as efficient retrofitting solutions. A variety of methods have been developed in this area. One method is the use of Finite Element Modeling (FEM) to study the behavior of a building during an earthquake. We used a program called ANSYS in this study, a multi-purpose finite element application that performs several types of dynamic analyses. In this study, modal and transient dynamic analyses are selected. The structure studied in this project is the Berkeley Town House located at 2550 Dana Street, built in 1961. The model is a three-dimensional, linear, isotropic finite element model based on the building. We then modified the structural support of the original model to see how it affects the response to seismic loads. In the building, only the northeast and southwest corners of the building are anchored to the foundation through the basement. The first modification was done by adding the same support columns from the southwest corner to the southeast corner, the second, adding the support columns to the northwest corner, and the third, adding the support columns to both the southeast and northwest corners. We analyzed the finite element models and studied their dynamic responses. The unmodified Original model produced a maximum stress of 12,206 psi. By comparing the maximum stresses of the original and modified models, we can see that the models highest maximum stress, 12,495 psi, occurs when the southeast support is installed alone. The maximum stress was greatly reduced to 9,881 psi when both southeast and northwest supports are installed. But the maximum stress is actually at its lowest of 9,823 psi when the northwest support is installed alone. By adding the support corners separately, we see that the southeast corner receives the most vibration and stress. This was determined by the increase in maximum stress when that corner was installed and thus made rigid and less flexible. Viewing the stress spectrum of the models, optimal areas to place the sensors would be in the four corners of the top floor, on the two basement corner supports and the ceiling of the basement right below the southeast northwest corners of the building as well.

Laser Ultrasonic Measurement of Elastic Properties of Metal Plates. *AMIR IRANMAHBOOB (Santa Monica College, Santa Monica, CA 90405) PAUL RIDGWAY (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

Laser ultrasonic analysis allows non-contact non-destructive measurements of mechanical properties of materials. Plate waves were generated in Aluminum 6061-T6 and AISI Stainless Steel 304 sheet using a pulsed CO₂ laser and were detected with a Mach-Zehnder interferometer. The plate wave phase velocity as a function of frequency was used

to calculate the flexural stiffness and shear rigidity of the metal samples. The values were then compared to expected values calculated from published elastic properties. The values were in agreement within experimental uncertainty.

Novel Methods in the Mitigation of Heat Trapping by Encapsulated Ballasts. *WILLIAM ROBBINS II (2ND) (Santa Barbara City College, Santa Barbara, CA 93109) MICHAEL SIMINOVITCH (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

Consumer confidence in a product is often entwined with the permanence of that product; energy-efficient technology is no different. The longevity of electronic ballasts for compact fluorescent lamps (CFLs) is often reduced by high operating temperature. By using the structures surrounding these devices as a heat sink, it is possible to curb the trapping of heat by the device and its enclosure. This goal is accomplished, most cost effectively, by a subtle alteration that can be made to popular recessed lighting fixtures during the manufacturing process; mounting the ballast enclosure to the pan. Simulations of long period, under extreme conditions were run in an isolated, superheated environment that was designed to emulate conditions found in the attic space of a home during times of peak temperature. The orientation of a prototype was varied to mimic possible implementation errors at the field level. In addition, to mimic possible environmental irregularities the experiments were tested with and without insulation covering the device. The experiments have shown a reduction in operating temperature of as much as ten degrees Celsius. The assurance of a long-life could help to boost consumer confidence and therefore, increase procurement and usage numbers of energy efficient, CFL based, recessed lighting by end-use consumers.

Spreadsheet Model of Yearly Furnace Electricity Consumption.

JEREMY COLEMAN (Monroe Community College, Rochester, NY 14611) JIM LUTZ (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Furnace gas consumption has long been an issue for standards and regulation for the US Department of Energy. It is only recently that some of the focus has begun to shift towards the issue of furnace electricity consumption, since furnaces are one of the highest consumers of electricity in residential households and there are currently no standards in place to regulate their efficiency. In order to better understand furnace power distribution during operation, a model was necessary to calculate furnace electrical consumption under various furnace configurations. This model calculates furnace electrical consumption with data inputted for a specific blower, motor, and duct system. It bases these calculations on input for heating degree days and cooling degree days for a specific location. In writing this model a good portion of time was dedicated to properly modeling the action of the blower in the furnace, since it is by far the largest consumer of electricity within the furnace, as well as being the most difficult component to accurately model. This work is mainly meant to promote an understanding of electricity consumption in furnaces, the tangible benefits being a useful tool in the future writing of furnace electricity standards and better understanding of how to modify and increase furnaces electrical efficiency.

Tobacco Related Disease Research Program Environmental Tobacco Smoke Collector Design. *KIMBERLY HINCKLEY (Georgia Institute of Technology, Atlanta, GA 30332) LARA GUNDEL (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

Exposure to airborne particulate matter (PM) and especially that produced by environmental tobacco smoke (ETS) has been linked to adverse health effects. However, the current methods of characterizing ETS exposure are potentially subject to misclassification bias. To address this bias, a simple exposure assessment device to quantify ETS exposure with PM, nicotine, and 3-ethyl pyridine (3-EP) measurements is being developed. The indicator will be free-standing, compact, and relatively inexpensive. It will consist of a passive gas collector and a particle collector. My work has focused on the device design in three areas: flow rate control, circuitry, and design ideas. A laptop fan was tested for the 15 cc/min flow necessary for thermophoretic forces. In conjunction with the fan, a hypodermic needle, acting as a critical orifice, supplies the desired stable flow. To help achieve the goal of a freestanding unit, I worked with a microcontroller, demonstrating its ability to control and log data associated with both the passive and particle collectors. Finally, I created computer renderings of design ideas of the final components, fixtures and housing. The fan assembly incorporates a luer fitting to accommodate the hypodermic needle. The passive collector includes three samplers and a means of switching between them, and a prototype has been machined. The final design houses both collectors, the flow control, circuitry, and power source into the shell of a camping lantern. This design work is crucial for a final durable,

freestanding, safe, list of adjectives and goals, indicator necessary for studies of ETS exposure.

TRAMS: Tracer-gas Airflow Measurement System. CRAIG JOHNSON (California State University, Chico, CA 95929) DUO (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Duct leakage has been identified as a major source of power loss in HVAC systems (Diamond et al, 2003). It is very difficult to measure this leakage and current standards do not give accurate duct leakage flow rates. Previous studies have identified flow hoods that can measure the airflow rate out of registers (Etur et al, 2003), but no system is currently available to measure the intake flows with the speed and accuracy required. The use of a tracer gas provides a simple and efficient method of measuring the airflow into the air distribution systems of large commercial buildings. Previous work was done using the tracer gas Sulfur hexafluoride (SF₆), but a faster and less expensive system was needed. The Tracer-gas Airflow Measurement System (TRAMS) developed uses Carbon dioxide (CO₂) as a tracer and provides a minimum accuracy of 1%. This is critical in order to make accurate measurements of duct leakage as small as 5%. TRAMS can accurately measure airflow rates from 5000 cubic feet per minute to 800 cfm. The system is designed to eliminate the need for a mass-flow controller by using an integration method to calculate the airflow rate. The CO₂ concentration is monitored using an infrared gas analyzer. The mass of CO₂ injected is determined by weighing lightweight CO₂ tanks before and after injection. Laboratory tests were performed on the system to develop the components and test its accuracy against a reference airflow meter.

Application of Engine Models and Vehicle Simulation Tools to Investigate Efficiency, Performance, and Emission Impacts of Advanced Engine Operation. DAVID MCCOLLUM (University of Tennessee, Knoxville, TN 37922) MATTHEW THORNTON (National Renewable Energy Laboratory, Golden, CO 89401).

The U.S. Department of Energy's (DOE) Office of FreedomCAR and Vehicle Technologies Program has developed a plan that outlines research and development needs for advanced petroleum- and non-petroleum-based fuels for on-road vehicle compression-ignition, direct-injection (CIDI) engines. The plan calls for developing and validating predictive models that will be used to set emissions targets for the program and pathways for realizing those targets. CIDI, "diesel," engines offer many advantages over traditional spark ignition (SI), "gasoline," engines. In this research project, two separate simulation tools, WAVE (a one-dimensional engine modeling software package) and ADVISOR 2002 (Advanced Vehicle Simulator), were used to study the efficiency, performance, and emissions impacts of advanced CIDI engine operation. WAVE was employed to create steady-state engine maps, which were later used in ADVISOR to simulate vehicle operation over different drive cycles. The focal point of the modeling was a 7.3-liter CIDI V-8 engine—specifically chosen because dynamometer-measured data for this engine was readily available. ADVISOR's steady-state engine map approach was validated by WAVE's transient simulation capabilities. Additionally, WAVE's ability to model an actual engine was assessed by comparing WAVE output to experimentally measured data. Lastly, several different engine efficiency and emissions control strategies (i.e., engine downsizing, adjusted valve timing, and cylinder deactivation) were investigated with WAVE and ADVISOR to determine their promise as a future, valuable technology. These simulations indicate that using a smaller engine and/or adjusting the valve timing have noticeable, positive effects on fuel economy and NO_x (NO and NO₂) and hydrocarbons (HC) emissions. Conversely, the simulation approach indicated that cylinder deactivation might have less promise in a CIDI application. Future work will focus on expanding the amount of empirical data on CIDI engines in passenger vehicle applications, and on improving the engine models to better predict NO_x and HC emissions of these engine/vehicle combinations.

Design of a Floating Wind Turbine Platform. ANDREW BOONE (Northern Arizona University, Flagstaff, AZ 86011) WALT MUSIAL (National Renewable Energy Laboratory, Golden, CO 89401). Deep water offshore wind sites may have distinct advantages over conventional land based and near shore wind sites. Resource studies indicate that wind speeds increase with the distance from shore, and the number of available deep water sites is enormous. Turbines located further offshore would not be visible from land, thus eliminating objections based on aesthetics. The problem of transmitting electrical power would be reduced compared to land based turbines because deep water wind turbines could still be located relatively close to large loads centers. In order to place wind turbines in deep water, floating wind turbine platforms must be developed. Initial studies of such platforms indicated that they would be prohibitively expensive to construct and install. For this project, the cost of a specific type of floating platform that had not previ-

ously been analyzed, called a tension leg platform (TLP), was estimated for a platform that would support a 5 MW wind turbine in water depths of 600 feet. This was a rough first-order cost estimation which did not include dynamic effects caused by varying wind and wave loads. MATLAB was used to solve the relevant quasi-static equations for the floating platform system and to find the dimensions of the optimal (lowest cost) platform. The platform was found to cost approximately between 3 and 6 million dollars per installed unit. A list of topics that should be researched in order to refine this estimate was compiled.

Developing a Small-Scale Multiple Generator Drive Train Computer Model. 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, which are necessary to generate power efficiently. 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 they have many other advantages, uncertainty about power sharing remains a primary concern. As a result, the National Wind Technology Center (NWTC) is considering building such a system and testing it on both its dynamometer, and on a small wind turbine. This paper documents the development of a MATLAB based computer model for use as a design tool, and for studying drive-train issues in torque sharing, vibration, power electronics, and control. The system contains models for a one-stage, three-output gearbox, three permanent magnet generators, a nine-phase diode rectifier, and a controllable DC bus. The functionality of each of these sub-systems was verified, and the components were assembled into a complete drive-train model. Drive train start-up, steady state operation, dynamic breaking, and faults were simulated. While many aspects of the model perform as expected, accuracy, stability, and robustness still needs to be improved.

Heteropolyacid and Poly(Vinylidene Fluoride) Pellet Membranes. DANIELLE HANSGEN (University of Washington, Seattle, WA 98105) JOHN TURNER (National Renewable Energy Laboratory, Golden, CO 89401).

Proton exchange membrane fuel cells are currently being looked at for several applications. Current operation temperatures are restricted to around 80°C because of hydration issues with the perfluorinated sulfonic acid polymer membranes. However, many fuel cell applications would benefit from the ability to run at higher temperatures - between 120°C to 150°C. We are examining the use of heteropolyacids in fuel cell membranes because they are stable at higher temperatures and have the ability to be good proton transport agents. A hot press was used to make pellet membranes that could be turned into membrane electrode assemblies and placed directly into the fuel cell to test the performance. The membranes were composed of heteropolyacid and an inert binder, poly(vinylidene fluoride). Membrane composition and production qualities were studied to find the optimal production conditions using Keggin- and Dawson- type phosphotungstate heteropolyanions. Performance was determined to be a function of: the time in the heat press, amount of the heteropolyacid, and the thickness of the pellet membrane. The best membrane, optimizing the previous conditions, was a Dawson-type diphosphotungstic acid membrane, producing currents over 200mA/cm².

Multiple Generator Drive Train Design for a Small-Scale Wind Turbine Test Bed. KEVIN SWEENEY (Northeastern University, Boston, MA 02115) JASON COTRELL (National Renewable Energy Laboratory, Golden, CO 89401).

Torque loads on wind turbine drive trains are becoming an apparent problem as the wind industry increases turbine size. One of the possible solutions to overcome this large amount of torque is a multiple generator design. Since the torque loadings are equally shared between generators, forces are more evenly distributed in the gearbox. This allows for a gearbox with larger tolerances and less structural strength to perform under the same torque load. With the reduction in weight and precision, the cost of energy (COE) of a commercial wind turbine is estimated to reduce by 12%. [1] In response to industrial trend of increase size of wind turbines, the National Wind Technology Center (NWTC) has interest in developing a small-scale wind turbine for testing of the multiple-generator drive train concept. The proto-type design would also incorporate the use of permanent magnet generators for their superior characteristics in high torque loadings. By developing a physical test bed for the multiple generator design concept the NWTC will be able to gain information on the suggested design in topics such as torque sharing, vibration, permanent magnet generators, controls, and power electronics. This paper explores the drive train options for retrofitting a 20 kW Grumman downwind wind turbine into a 32 kW multiple genera-

for design. Industry drive train trends are studied and are evaluated for this particular project. A comparison between two finalized drive train designs are evaluated based on functionality and cost. The recommended design for this wind turbine uses a turntable bearing design. It can be easily maintained, and modified if needed. The turntable bearing application will offer an effective solution and will have a 59% reduction in cost when compared to the cast gearbox design.

Native American Renewable Energy Approaches: Navajo Tribal Utility Authority and Native Sun. KEITH CANDELARIA (*Dartmouth College, Hanover, NH 03755*) SANDRA BEGAY-CAMPBELL (*National Renewable Energy Laboratory, Golden, CO 89401*).

Native American tribes encounter many new technologies today, some of which may positively or negatively affect the lives of their people. One area where technology is growing is the renewable energy field. Depending on where a tribe is located, the tribes may have options to explore new technologies that are available. Many issues and concerns affect the decisions of tribes because the tribal leaders understand that the decisions they make today will definitely affect the future generations of their people. This paper focuses on two tribes, the Navajo Nation and the Hopi Pueblo. These tribes have taken steps toward using photovoltaic systems to provide electricity for their communities. The two businesses that have made the solar programs successful within these tribes are the Navajo Tribal Utility Authority and Native Sun. These solar programs were made possible by champions within the tribes that worked towards what they believed in. These champions are needed to sustain the programs so that they may continue to be successful in assisting the needs of the tribal members.

Navajo Tribal Utility Authority: Electrification Demonstration Program Developing a Sustainable Tribal and Rural Cooperative Solar Program. SHAUN TSABETSAYE (*University of New Mexico, Albuquerque, NM 87131*) SANDRA BEGAY-CAMPBELL (*National Renewable Energy Laboratory, Golden, CO 89401*).

There is a lack of electricity on approximately 18,000 off-grid homes on the Navajo Nation because of isolation and lack of electrical grids available. The Navajo Electrification Demonstration Program (NEDP) was created and funded in 2001 by Congressional appropriation to be implemented by the Navajo Tribal Utility Authority (NTUA), a 30-year-old rural utility co-op. The NEDP allows for 50% of the 3 million dollar annual appropriation to be used to electrify off-grid homes with 880-watt photovoltaic (PV) /15-watt wind hybrid systems to use solar and wind technologies. The ultimate goal of my work is to help the Navajo Nation and NTUA sustain a solar energy program as a viable technology option for the Navajo. NTUA can also serve as a model for sustainable solar energy development for tribal governments and rural utility co-ops. As a result of my work, NTUA has a baseline to standardize procedures and workflow methods across 7 districts and retains the ownership of my work and may modify the procedures to their needs.

NREL Wind Site Entrance Building Examination. WALTON WARD (*Massachusetts Institute of Technology, Cambridge, MA 02139*) PAUL TORCELLINI (*National Renewable Energy Laboratory, Golden, CO 89401*).

The National Wind Technology Center (NWTC) had a site entrance building (SEB) constructed following the September 11, 2001 attacks for added security. The SEB was designed by the National Renewable Energy Laboratory's (NREL) High-Performance Building Design Team. The goal was to design a building that would not be dependent on the power grid on a yearly scale: a net zero-energy building. This would be done through renewable sources, such as photovoltaic panels, wind turbines, passive solar heating, daylighting, and other technologies. Currently, the building is a fully-operational center for the NWTC's security needs. The SEB is 30% more energy efficient than other similar security buildings. In addition to its energy savings, the onboard renewable power sources supplied 43% of the building's energy needs in the first half of 2003. Although the building uses a small amount of energy from the grid, its ultimate zero-energy goal has not been attained. The purpose of the research is to use a computer simulation program called SUNREL to analyze the efficiency of the building and give recommendations for improving the performance of the SEB. During the research, simulation results were compared to measured performance data in order to calibrate the simulation and to fix inefficiencies in the SEB. Our tests showed that covering the Trombe wall, a thermally conductive wall that provides heat to the building in the winter, during the warmer months reduced energy costs for cooling the building up to 66%. Also, disabling the SEB's occupancy sensor, which controls the lighting and heat pump, will help to reduce energy costs and create a more comfortable and stable working environment. The final recommendation involves installing a second wind turbine that was included in the original building

plans. These three recommendations will potentially upgrade the SEB to a zero-energy status.

Reducing Benzene Levels in National Renewable Energy Laboratory's. MICHELE BUZEK (*University of Colorado at Boulder, Boulder, CO 80309*) STEVEN PHILLIPS (*National Renewable Energy Laboratory, Golden, CO 89401*).

The Thermochemical Process Development Unit at National Renewable Energy Laboratory converts biomass into energy by gasification or pyrolysis. The aqueous effluent generated in these processes must be disposed of as hazardous waste according to the Resource Conservation and Recovery Act because certain components of the scrubber water are regulated and exceed the concentration limit. Gas stripping was investigated as a method of reducing the benzene levels in the scrubber water. A custom-designed packed-bed column was built and a half-factorial experimental design was implemented to determine the effects of gas flow rate, liquid flow rate, and column packing height on the final benzene concentration in the liquid. The experimental results show that packing height had a significant effect on final benzene concentration; gas flow rate and liquid flow rate had little effect. Although the current column design did significantly reduce the benzene levels in the scrubber water, it did not reduce the benzene levels below the stated limit. A full-factorial experimental design will be implemented with an increased packing height. Other variables, including column diameter and packing, will be investigated to determine their effects on final benzene concentration. Once the packed-bed column is determined to be effective in removing the benzene from the scrubber water, and reducing the concentration below the stated limit, photocatalytic oxidation will be explored for remediating the benzene from the gas steam.

Thickness Measurement of Silicon Wafers Using the PV-Reflectometer. A. CHRIS AURIEMMA (*City College of San Francisco, San Francisco, CA 94112*) BHUSAN SOPORI (*National Renewable Energy Laboratory, Golden, CO 89401*).

The U.S. photovoltaic cell (PV) industry has sufficient production volume to warrant a move to process monitoring, but currently lacks monitoring devices appropriate for solar cells. The PV Reflectometer has the potential to provide the PV industry with fast, cost-effective, real-time monitoring of solar cell parameters. Of these parameters, silicon wafers thickness is one of the most important because it directly affects the performance of solar cells both in production and in the field. The thickness measurement capabilities of the PV Reflectometer rely on the thickness dependency of reflectance in a wavelength range where light is reflected from both the front and back sides of the silicon wafer. In this range, thicker wafers are predicted to have lower reflectance than thinner wafers. The original goal of this project was to compare standard thickness measurement techniques with measurements made with the PV Reflectometer. Ultimately this comparison was not possible due to irregularities in the surface characteristics of the wafer available for testing. As a result, the present paper presents a proof of concept for thickness measurement using the PV Reflectometer and an investigation of the problems encountered during the research. The data, consisting of reflectance vs. wavelength curves, was generated for single and multi-crystalline silicon wafers as well as EFG ribbon wafers. The same wafers were measured using three standard techniques, in particular, mass measurement, dial gage and use of a capacitance-based electronic device. Results show that for rough and textured single and multi-crystalline wafers the PV Reflectometer produces similar curves for wafers of the same or similar thickness. For these samples, in the appropriate wavelength range, reflectance is lower for thicker wafers, as predicted by optical theory. The results for ribbon wafers did not conform to theory, due to variable surface characteristics. Further testing will be necessary empirically demonstrate the conversion of raw data into thickness values and to investigate surface variation issues, particularly with respect to ribbon wafers.

Time Series Optimization of Hybrid Wind Systems. FRANK MALDONADO (*University of New Mexico, Albuquerque, NM 87110*) LEE JAY FINGERSH (*National Renewable Energy Laboratory, Golden, CO 89401*).

Hybrid wind-hydrogen systems show promise as a future source of clean, renewable energy. Combining the strengths of wind and hydrogen, it is possible to create a reliable energy source to supply energy to the electrical grid, offset conventional generation, and produce excess hydrogen for other markets. In order to accomplish this, the optimization of several devices is required. In addition to the wind turbines, fuel cells (devices that use hydrogen and oxygen to produce electricity and water), electrolyzers (devices that convert water and electricity into hydrogen and oxygen), and battery storage must be utilized. Creating a control structure to make the best use of each component and reduce the overall system cost is key in building an effective system. Using

the modeling spreadsheet application WindSTORM, control algorithms were developed to supply power to the electrical grid while utilizing the hybrid system to reduce conventional generation. The analysis of this study shows there is much potential for this system to be an effective energy alternative in the future. The model was able to significantly reduce the required capacity of conventional generation, and may be further reduced with continued development. This study provides a framework to build upon in the future, as there are multiple areas to be addressed in order to have a more complete assessment of the hybrid wind-hydrogen system.

Wind Tunnel Tests on Tabbed Fins. MATTHEW DUBROVICH (*Lehigh University, Bethlehem, PA 18015*) CHUCK KUTSCHER (*National Renewable Energy Laboratory, Golden, CO 89401*).

This research project aimed to further study a unique, recently developed fin design for air-cooled condensers such as those used on geothermal power plants. The design incorporates a system of 'tabs' that are bent outward from the fin and into the air stream. Previous research has shown large improvements in the heat transfer coefficient when a simple grid of tabs is used on a set of fins. Also the pressure drop increase due to the tabs was not large. This project used a more complex experimental setup that consisted of multiple heat exchanger tubes passing through the set of fins. Unexpected problems arose during testing and only pressure drop data from different fin configurations have been recorded. Tabbed fins with a spacing of 5 fins per inch (FPI) had a pressure drop increase of 32% over plain fins while tabbed fins at 10 FPI had an increase of 58%. These results are promising and more research into tabbed fins is suggested.

A Thermal Mass Benefit Calculator. AARON KEEGAN (*Warren Wilson College, Swannanoa, NC 28778*) JAN KOSNY (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Studies dating from the energy crisis of the 1970's to the present day have shown that buildings with exterior walls constructed from massive materials can achieve lower heating and cooling energy demands than buildings with comparable walls of light-weight construction. For a given home, determining the quantity of savings that could be achieved from massive walls requires field experimentation and/or whole building energy simulation. These methods are often too time consuming to be included in the construction planning process. In an effort to reduce the time necessary to determine the potential energy savings of a massive wall system, a simplified calculation tool was created. Data was obtained from a massive wall system study performed by J. Kosny et al. in 2001. Regression analyses were performed on multiple data fields including heating load, cooling load, electricity consumption, natural gas consumption, and total energy consumption. The regression equations were then programmed into a graphical user interface program written in Visual Basic. The result is a prototype application that allows users to compare the energy performance of four different massive exterior wall configurations to a wood frame exterior wall. Comparisons can be made for three model homes in 10 U.S. locations. The program will benefit from further development as more locations, home models, and climate control system options are added. The program will eventually be deployed on Oak Ridge National Laboratory's Building Envelopes Program website for public utilization.

Analysis and Calibration of Side Emissions for Development of new Control system. SCOTT STELLERN (*Clemson University, Clemson, SC 29634*) D. L. BESHEARS (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The Hybrid Lighting project combines the use of solar collection and remote source lighting. A hybrid light fixture combines fluorescent light with natural sunlight. This conserves energy and the natural light helps provide a friendlier atmosphere. To maintain a constant light level, a photometric Li-cor sensor is placed in the center of the room to monitor light levels and make adjustments. Presently, to measure the amount of light a fiber is emitting an integrating sphere must be used. A new system involving photometric light sensors attached to the fibers themselves would eliminate the need for an integrating sphere, which can be hard and time-consuming to use. The integrating sphere was used to measure light levels of a specific fiber, which was then compared to the measurements of a photometric Li-cor sensor attached to the side of the fiber. After comparing these two measurements, a formula was made to relate the measurements. It was discovered that the relationship was linear and that the side emission is a simple percentage of the total light emission. Now to monitor the amount of light a fiber is emitting, a simple side sensor can be attached to the fiber and a few calculations can be done. This will help monitor each fiber for defects and deterioration, which will help conserve energy, the ultimate goal of this project.

Application of Phosphor Thermometry to Fuel Cell Diagnostic.

DUSTIN GARVEY (*University of Tennessee, Knoxville, TN 37916*) STEVE ALLISON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Phosphors are most generally described as rare earth doped materials that emit fluorescence when properly excited. This fluorescence may have several temperature dependant characteristics. One of the more temperature sensitive characteristics is the decay time. Measuring and comparing decay times to known calibrations allows very precise temperature measurements to be made. This method is to be applied to fuel cells. The main requirements for this detector are a low cost and a measurement range from 40 - 150°C. In order to satisfy the cost aspect, light emitting diodes (LED) have been chosen to excite the phosphor. By bundling varying numbers of 400-micrometer diameter optical fibers and directing them toward an LED, it was found that fluorescence was obtainable from a YAG:Cr sample using each of the fibers contained in the largest bundle (35-fibers) for excitation. This result establishes that it is possible to use one LED for many individual thermal detectors (35 demonstrated), which lowers the cost even further. To lower detection cost, a photodiode (PD) should be used in the future to replace the more expensive photomultiplier tube (PMT). Because a PD has a smaller gain than a PMT, a phosphor with a very intense fluorescence must be used. Small diameter ruby spheres have proven to be the best candidate. They have emitted a 1.4 V fluorescence signal, which is significantly larger than the 0.35 V signal from the YAG:Cr. Using the various LEDs that were available in the lab (370, 395, 405, 430, and 450 nm), a limited excitation spectrum has been made of the ruby in order to choose the LED that maximizes ruby excitation. It was found that the ruby is most excited by a 405 nm LED. Next, varying resistances were used to measure the fluorescence. The larger the measurement resistance, the stronger the fluorescence and the more distorted the decay time. Through comparative analysis it was found that the measurement resistance could be on the order of 26 k Ω with no significant distortion in the decay time ($\pm 2\%$). The collected data represents the bounds that limit the design of the thermal detector and will aid in future design decisions.

Building Integrated Photovoltaics On Low-Slope Commercial Buildings.

EDMUND BROWN (*San Juan College, Farmington, NM 87401*) WILLIAM A MILLER (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Documentation of the benefit of Building Integrated Photovoltaic's (BIPV) effect on mitigating building cooling load and roofing system performance is sparse. Roofing contractors, architects, photovoltaic (PV) manufacturers, builders and utilities are asking for this data to increase their understanding of building system performance and to quantify building load energy savings. Creating a rating procedure to compare the energy efficiency of a roof that integrates PV equipment with the efficiency of a conventional insulated roof, is the objective of a project under way at The Building Technology Center (BTC) at Oak Ridge National Laboratory (ORNL). Two ongoing programs at the BTC provide a unique opportunity to conduct the research required to quantify the impact of BIPV on building cooling and heating loads. One program involves a partnership among the Federal Energy Management Program (FEMP), the Tennessee Valley Authority (TVA), British Petroleum (BP), the ORNL State Partnership Program, and the State Energy Office (SEO). An array of 72 polycrystalline panels are installed on the roof and south wall of the Envelope Systems Research Apparatus (ESRA). The second program involves the testing of a laminate amorphous silicon material on the ESRA - a roofing test facility with just about every material used in low-slope roofing installed on the roof. Extensive historical data is available from both these programs including climatic, roof and BIPV temperature and heat flow, and solar system performance data. This project is focused on the consolidation and validation of the data, from the above mentioned sources, into a single database and the creation and validation of the roof performance rating system. To create and test the rating system, this data is input to a BTC created roof system model that predicts heat flow and temperature within the roof. This model is called STAR - Simplified Transient Analysis of Roofs. Actual measured data is compared to the predictions of STAR to validate the rating procedure. The rating system has been tested and it performs well. The rating system can now be used to predict the performance of roofing systems and the impact of BIPV on building heating and cooling loads in various locations around the country.

Characterization and Properties of Aluminum Lithium Alloy 2195 Friction Stir Weld.

JACOB DAWSON (*South Dakota School of Mines and Technology, Rapid City, SD 57701*) STAN DAVID (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Aluminum-Lithium alloy 2195 is being used in constructing the external

tank of the space shuttle for several reasons including a high strength to weight ratio. However, like many aluminum alloys the material is difficult to fusion weld. Friction stir welding is being explored as a possible alternative to fusion welding. Flow properties (mechanical properties) of the friction stir weld zones including the weld nugget, thermomechanically affected zone (TMAZ), and heat affected zone (HAZ), as well as the base material were studied in this experiment. The flow properties of each relatively small zone were determined through a new nondestructive and localized testing method called Automated Ball Indentation (ABI) testing. The HAZ exhibited the lowest yield strength and UTS. Flow properties of the weld nugget and TMAZ were very similar to one another. However, the strengths throughout the weld region were lower than the base material. Decrease in strength of the friction stir weld is mainly due to metallurgical changes that arise from the thermal cycle experienced by the material during the weld. As the strengths decrease through friction stir welding, the uniform ductility of the material is increased. Uniform ductility was found to be ~6% in the base material and ~12% in the weld area. Future work will include fracture toughness experiments as well as attempting to strengthen the weld through precipitation hardening. Fracture toughness measurements are of special interest at cryogenic temperatures required to store liquid hydrogen and liquid oxygen, which serve as propellants for the space shuttle.

Computational Modeling of Bifurcated Abdominal Aortic Aneurysms. JENNIFER LILLY (*University of Tennessee, Knoxville, Knoxville, TN 37916*) KARA KRUSE (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

New developments in research have strived to model abdominal aortic aneurysms (AAA) by integrating computed tomography (CT) scans, segmenting software and finite element (FE) analysis. AAA has troubled the medical field in the past due to the lack in development of an accurate means of diagnosis. The high mortality rates in cases where the patient experiences a rupture have been the primary motivation in developing new and improved methods to determine where the point of rupture is likely to occur. Developing a proper means of estimating the distribution of stress in an AAA would be advantageous in predicting whether an aneurysm has a high probability to rupture. Fundamental to this process is creating a model that is appropriate for both the wall and the intraluminal thrombus found in AAA. Past case studies on AAA have neglected to include cases that account for the bifurcation in the aorta, the point at which the aorta separates into the two femoral arteries. Previous software has been limited in producing a viable model of the bifurcated aneurysm that would be capable of producing reasonable results in finite element analysis. New improvements in currently available commercial software have led to the more in depth investigational studies and applications. Various programs have been undergoing evaluations in order to determine which would be most efficient in segmenting the AAA and creating a representational 3D model of the bifurcation. At this time there is no conclusive evidence as to which program performs the tasks at hand superior to another. However, one particular program, Amira 3.0, has been utilized extensively and shows potential promise. This program successfully segmented the AAA from the patient CT data and created a 3D model. Currently, a model has yet to be created that is sufficiently smooth enough to be imported into the finite element program in order to create a mesh. It is expected that a model will be produced that is capable of creating a representable mesh of the surface of the model, at which stress analysis may be conducted in order to determine areas of significant pressure occurrences. Once these high-pressure areas are determined, the quantitative data will be compared with the known point of rupture from the vascular surgeon who handled the particular case in study. This comparison will aid in the determination of the accuracy and precision of the model and stress analysis.

Development of Modeling Techniques for Abdominal Aortic Aneurysms that Include the Bifurcation of the Aorta. STEPHANIE BARNES (*University of Tennessee, Knoxville, Knoxville, TN 37916*) KARA KRUSE (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*). Abdominal Aortic Aneurysms (AAA) are a serious problem for the medical community; often the end result is the death of the patient, as there is no truly successful way to treat AAAs after rupture. The best way to treat an AAA is to prevent rupture. Developing a means by which the rupture point of an AAA could be determined could advance the procedural treatment of AAAs. Research has been done utilizing computerized tomography (CT) scans as the basis for creating a 3D model of the AAA, which can then be tested to determine the points of elevated stress and to predict potential rupture sites. CT scans are often taken of patients with AAAs to determine the extent of their distress; they provide visualization of the outer wall of the aorta, the inner lumen, and the thrombus, as one progresses down the aorta, which makes them

beneficial for modeling purposes. The previous research proved very successful; the point of rupture that the model predicted coincided with the actual point of rupture. Current research focuses on the CT scans of a patient with an AAA that ruptured approximately 3 days after the scans were taken. The difficulty with this particular AAA is that it encompasses the bifurcation, where the aorta divides into the two iliac arteries, whereas the AAAs from the previous research did not incorporate the bifurcation. Previous methods for modeling the AAA did not allow for inclusion of the bifurcation; thus a method had to be devised to successfully model the bifurcation. Testing is in process to determine which of various programs would be most beneficial and accurate in segmenting the AAA and visualizing the bifurcation in a 3D model. Though it has not yet been determined which program will prove the most successful, one of these programs, Amira, has been utilized for further testing. The CT data was segmented and a 3D model was created employing Amira. This model was then imported into an NURBS geometry program, which was used to modify and improve the geometry of the bifurcation. The model was then imported into a geometry-meshing program, which created a mesh on the surface of the model; the surface proved meshable, which is an important requirement of the model. The next step includes the model being put through a finite element analysis to determine the points of high pressure in the AAA. These determined points will then be compared with the known point of rupture to assess the accuracy of the model and the modeling techniques.

Energy and Demand Savings from a Geothermal Heat Pump Retrofit in Military Residences in the Southeastern United States. ANTHONY FLORITA (*University of Wyoming, Laramie, WY 82070*) JOHN SHONDER (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*). At a military base in the Southeastern United States, air-source heat pumps were replaced with geothermal heat pumps (GHPs) in more than 2,000 family housing units. Because GHPs exchange heat with the earth instead of with ambient air, they have the potential to make significant reductions in energy use compared with air-source equipment. Ground temperatures do not vary as extensively as the temperature of the ambient air over the course of the year, which allows GHPs to maintain stable heating and cooling capacity and to operate more efficiently. The objective of this paper is to assess the design of the project and to determine the energy and demand savings that have resulted from the retrofits. Energy usage was calculated by correlating measured energy data with total degree days. The correlation between monthly extreme temperatures and peak energy demand was used to find demand savings. Linear regression techniques were utilized in both cases to identify comparable equations and find pre- and post-retrofit savings. The savings calculations are complicated by the fact that the available utility bills measure electrical use in the entire family housing stock, which includes about 4,000 homes. It was found that the GHPs reduced energy use by 30%, which compares well with other projects. Demand saving was on the order of 10%. One potential problem with the design is that the ground heat-exchangers may have been undersized in some residences. Anthony Florita University of Wyoming John Shonder Engineering Science and Technology Science Undergraduate Laboratory Internship (SULI)

Evaluation of Candidate High Temperature Phosphor Binders. NOAH BERGERON (*University of Louisiana at Lafayette, Lafayette, LA 70504*) STEPHEN W. ALLISON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Fluorescence from phosphor materials offers a method of non-contact thermometry in hostile environments such as those found in high temperature regimes (1200-1700°C). Phosphors are typically rare earth doped ceramics that emit light when excited. The intensity, rise time, decay time, and wavelength shift of this emitted light can be temperature dependent. If thermographic phosphors are applied to a surface, an excitation source and a method to characterize the emission are provided; it is possible to determine a temperature of the surface. The coating method involved in this study is the use of phosphor paints. These temperature sensitive paints are created by mixing phosphor with a binder material to form a sprayable coating that can be easily and economically applied to a large area. Given that decay time calibration data exists to 1700°C, it is desirable to have phosphor paints that will survive to at least that temperature. The survivability of phosphor paint depends on characteristics of the binder. The goal is to discover binders that will allow phosphor paints to survive to high temperatures. Binders that survive to high temperatures will allow for the construction of non-contact measurement devices useful in environments that are not suited for more common thermocouple or infrared devices. For a phosphor paint to be useful at a certain temperature the paint must fluoresce when excited and decay time must be measurable. In this study, Cotronics Resbond 791, 792, 793, 794, and 795 ceramic binders

were evaluated to determine their suitability for serving as phosphor binders with Y2O3: Eu. Post-thermal cycling spectral analysis was used to quantify wavelength and intensity changes in emission from UV excitation. Several of the paints utilizing their binders were able to survive temperatures of 1500°C. It is hoped that the results of this research will lead to studies involving the use of phosphor/binder paints in rocket-based research.

Evaluation of *in vitro* Canine Abdominal Aortic Aneurysm via Finite Element Analysis. JOEL OUTTEN (*University of Tennessee, Knoxville, TN 37916*) KARA KRUSE (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

There is a great scientific effort aimed at quantifying endotension in abdominal aortic aneurysm (AAA). Finite element analysis (FEA) has been utilized to computationally model endotension, but there has been no comparison with experimentally determined data to validate stress measurements within the aneurysm sac (AS). A previous experiment entailed taking pressure measurements, via diaphragm pressure transducers, within the AS of three *in vitro* canine AAA specimens. Pressure measurements were taken at eight distinct locations within each specimen. The goal of this study was to generate FE models of the three canine abdominal aortas and compare the computational stress measurements at the transducer sites with the experimental data. Computed tomography (CT) images were used to construct the models, which were subsequently meshed into finite elements. The models consisted of three different sections: AAA wall, intraluminal thrombus, and the stent-graft. The ends of the models were fixed in the axial direction in an effort to simulate the experimental set-up, and a constant, uniform, intraluminal pressure was applied. Each canine model was run at intraluminal pressures of 85, 100, and 120 mmHg. Element sets were defined at the locations of the experimentally utilized pressure transducers, and an average stress was calculated for each set in the direction normal to the transducer diaphragm. The computational stress was only weakly correlated to the experimental pressure for one model, while the other two were uncorrelated. While FEA failed to correctly model the pressure measurements, this work presents a new method of FE validation for AAA modeling.

Future Combat System Combat Identification Speed of Service

Model. LAUREN HATCHELL (*Louisiana State University, Baton Rouge, LA 70803*) GLENN ALLGOOD (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

DARPA's Future Combat System (FCS) Integrated Support Team has developed a Combat Identification (CID) notional architecture for Increment I FCS. Combat identification is the process of identifying entities in the battle space for purpose of fratricide reduction and increased combat effectiveness. CID solutions must include ground-to-ground, ground-to-air, and air-to-ground elements. In support of the air-to-ground element - Fixed Wing to Ground CID - a 'speed of service?' model has been developed using queuing and renewal theory to provide an analysis of latency and quality of service in the FCS communication network. The application of queuing and renewal theory eliminates the conditional dependencies of one node to another, reducing model overhead. Latency is described in terms of Time-to-ID based on the following model: propagation time, transponder processing, interrogator message identification and reformatting, data links to command and control (C2), C2 message identification and reformatting, human decision, and data links to shooter. The model also allows for a re-task decision at the C2 level. Algorithms have been developed that provide closed- and open-form probability density function solutions. The closed-form solution is derived by convolving input functions, while the open-form solution is derived from a simulation that yields an array of data points. In the future, the model will allow for the input of specific platform variables (aircraft, radar, sensor). Although originally developed for Fixed Wing to Ground, the speed of service model can be extended to ground-to-ground and ground-to-air situations. The model is flexible in that it will allow for many scenarios, network configurations, and sensor-shooter links. Subject matter experts have been consulted to determine reasonable input functions for a non line-of-sight (NLOS) situation. Results of the Fixed Wing to Ground NLOS simulation fall within a thirty second Time-to-ID requirement, but in a re-task scenario Time-to-ID exceeds the requirement by as much as twelve seconds. However, uncertainty in the network configurations may lead to longer latency times. Future plans include acquiring more information on the network links to confirm an NLOS Time-to-ID latency. Intelligent agent software will be developed that will reduce latencies and make the information more useful by abstracting large amounts of information and analyzing the quality of service of the networks.

Gas-Phase Mercury Separation Involving Room-Temperature Ionic Liquids. CHRISTOPHER HARRIS (*Texas A&M University, College Station, TX 77843*) DAVID DEPAOLI (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The discovery of toxic mercury in many areas throughout the United States has recently increased scrutiny of coal-fired power plants, the largest source of anthropogenic mercury emissions. Coupled with the pending EPA regulations on mercury emissions, a pressing need exists for efficient mercury removal technology. Previous experiments have proven room-temperature ionic liquids (RTILs), "green solvent" salts that possess negligible vapor pressure and are molten below 100°C, to be effective chemical agents for catalysis, metal extraction, and gas separation. The goal of this research was to experimentally determine the suitability of mercury-specific RTILs for mercury removal from a gas stream. The bench-scale experiments pass redox-generated mercury vapor past a semi-permeable membrane coated with RTILs. A time-of-flight mass spectrometer detects changes in the temporal response of the mercury signal as mercury is removed from the gas stream and absorbed by the RTIL. Preliminary results indicate that two of the ionic liquids studied create up to a thirty percent mercury reduction of mercury in the gas, while one reduces values in excess of ninety-nine percent, suggesting the further evaluation of their use for mercury removal. Future research will be focused on RTIL optimization, application, and mercury and ionic liquid recovery. This research is part of an ongoing collaborative effort to reduce toxic contents from flue gas and other emission sources by using ionic liquid separation technology.

Improving Existing Homes for Energy Efficiency. KIMBERLY HULVEY (*University of Tennessee at Chattanooga, Chattanooga, TN 37403*) THERESE STOVALL (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Energy efficiency is a growing concern for people around the world. Conserving energy will not only save consumers money but also ensure a better environment for the future. Energy is transferred in the form of heat through walls and windows of homes by conduction, convection, and radiation. Conduction is energy transmitted between two areas by the transfer of kinetic energy. Convection is heat transfer by fluid movement, and radiation involves waves of energy. To make homes more energy efficient, these methods of heat transfer need to be minimized. Existing products are being tested to help consumers select the best energy efficient products for their homes. The goal of this research is to increase ventilation and decrease infiltration. Ventilation is the process of providing adequate indoor air quality. Infiltration is the movement of outdoor air in and out of the inside of a building through inadvertent openings. Tests were done on an 8 ft x 8 ft wall with a window to determine thermal resistance using the Rotatable Guarded Hot Box test facility. Various insulation materials were applied to this wall and window in order to determine the best products for certain climates. Air leakage was characterized by regressing airflow rates against pressure differences. This characterization can then be used to predict infiltration for various environmental conditions. The test results were analyzed and used to develop a building simulation model employing the DOE 2.1E program. This model then estimated whole-building energy consumption for three sizes of homes in ten cities across the United States. Heating and cooling savings will be analyzed from this output. A summarized form of this data will be included in a consumer's guide to improving existing homes for energy conservation and savings. Previous work done on windows was also reviewed and will be included in the consumer's guide.

Investigation of a Rotating Arc Spark Plug (RASP) for Use in Stationary Power Lean Burn Natural Gas Engines. MARK BENNETT (*University of Kentucky, Lexington, KY 40506*) JOHN WHEALTON, JOHN ANDRIULLI (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

As our nation's energy demand increases, less efficient power plants may be forced back into operation and result in a negative environmental impact. Natural gas is a relatively 'clean' fuel source while alternative technologies are being investigated. The Rotating Arc Spark Plug (RASP) has potential benefits in helping the Advanced Reciprocating Engine Systems (ARES) program achieve efficiency goals by reducing cycle-to-cycle ignition variation, improving ignitability by increasing arc volume, reducing electrode erosion by the moving arc sites, and improving ignitability by means of higher plasma electron temperature. In theory, an axial magnetic field imposed on a radial gap spark plug will cause the radial arc to rotate circumferentially by the Lorentz force. The amount of rotation depends on the magnetic field strength (produced by high temperature permanent magnets), the current amplitude, and the duration of the spark. To investigate RASP potentials a high-speed camera capable of capturing 10,000 frames/sec is used to observe a single

arc from each RASP tested. The spark plug arc can then be viewed at various points in time to determine amount of rotation and rotation velocity at pre-combustion pressures. The RASP will then undergo thermal testing in a natural gas test engine at various loads. Upon successful thermal testing an in-cylinder combustion pressure gage will be used to compare the RASP design to that of a conventional spark plug by measuring the pressure pulse variation from cycle-to-cycle. Monitoring the combustion pressure pulses and other performance parameters will also allow for optimization of engine control systems. If the RASP design shows less pressure pulse variation, increased combustion pressures, then the possibility of a leaner air/fuel mixture may be used to produce the same amount of power with higher fuel efficiency and lower exhaust emissions. Future work will include research into new materials for longer lasting spark plug electrodes, higher temperature magnets, and comparison testing.

Modeling of Antenna Structures for Implantable Monitoring Systems. CHARYMAR CINTRON (*University of Puerto Rico, Mayaguez, PR 00714*) PAUL D. EWING (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The interest in knowing how electromagnetic (EM) waves and fields affect our bodies has become a popular field of study during the last few years due to the fast proliferation of cellular telephones and other electronic devices. Stemming from this point, the purpose of this project is to model different kinds of antenna structures for an implantable monitoring system. These antennas will be implanted in a simulation model of a human body to determine the radiation and efficiency of the antenna as well as the specific absorption ratio (SAR) of the surrounding tissue. The different antenna structures that have been modeled are the monopole antenna, the electric dipole antenna and the loop antenna. In order to develop these models, a software named REMCOM was used. This software uses the Finite Difference Time Domain method (FDTD) to predict the performance of the radiating devices and provide an accurate prediction of the interaction of EM fields with biological tissues. Simulations will be performed using antenna structures implanted in a human abdomen model with a focus on antenna transmission efficiency and SAR. The greatest challenge of this work has been to struggle with the complex nature of human tissues and with the reduced size of the antennas. This work is part of a DOE-funded research program developing implantable electronics for real-time tissue perfusion monitoring.

Monocular Visual Servo Tracking Control of a Wheeled Mobile Robot. ERIC HOLCOMBE (*Clemson University, Clemson, SC 29632*) WARREN DIXON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Motivated by the desire to navigate a wheeled mobile robot (WMR) without the requirement for multiple sensors or cameras, a new control strategy was recently developed that utilizes a single camera for autonomous navigation. The controller uses multiple views by a single camera to recover depth information through a Euclidean homography (a geometric relationship). Performance of this controller was previously demonstrated via a MATLAB simulation. The goal of the current project is to construct a proof-of-principle robotic testbed and implement the control theory. Preparations for the testbed included integrating specialized camera and computing with the WMR, building a target, and implementing the simulation in C/C++ for execution on the QNX real-time operating system. Converting the simulation code involved making a server program for live image processing and calculations and another program that would make calculations from recorded images. Additionally, code that employs the kinematic aspects of the controller was written and designed for execution by a program created for directly controlling robots with variable tracking and tuning capabilities. For the server code, an algorithm was developed to scan image frames for the necessary image feature information. The server program would then use the image feature coordinates to compute the translation and rotation information that was then transmitted to the main WMR computer. The results of this project are that a control strategy was demonstrated to force a WMR to navigate along a prerecorded image trajectory via feedback from a monocular camera system.

Partial Discharge in Voids in Epoxy as a Function of Pressure. 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 potentially catastrophic, costly, and unforeseen failure. Therefore, understanding PD and its causes can help diagnose problems and predict the expected lifetime of a dielectric. For insula-

tion 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 void that forms as a bubble in the curing of an epoxy dielectric. To study the onset and pattern of PD, and to better diagnose electric insulation in general, two samples were prepared with artificial voids embedded in dielectric epoxy between parallel plane electrodes. The samples were also designed in such a way that the pressure in the voids could be varied. The PD onset was then investigated as a function of pressure in the void using Nitrogen and Sulfur Hexafluoride gas. 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) we were able to capture the PD pattern. Different PD onsets are observed as the pressure is varied for the two systems. The onset voltage generally follows the Paschen curve dependence on pressure for each gas. These samples were then modeled using the program FemLab to better determine the electric field of the sample and how this field affects PD. In order to help clarify the PD signals originating from the sample, and the significance the pressure in the void has on the PD, the general pattern of PD will be discussed, along with the importance of the dimensions of the void and how they affect the electric field in the sample. Some suggested mechanisms for the observed PD patterns will also be discussed.

Quantitative comparison of optical efficiency and spatial intensity distribution of dual hybrid luminaire designs. DAVID REED (*Virginia Polytechnic Institute and State University, Blacksburg, VA 24061*) JEFF MUHS (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Sociological influences have advanced the concern for more practical methods in energy consumption. Hybrid Solar Lighting incorporates the direct power of natural solar energy and the widespread energy efficient florescent lighting systems to deliver an advanced form of lighting that offers many benefits to its end users. First generation luminaires were designed to show project feasibility, but as the second-generation solar collector evolves, the need for more efficient luminaires has become an important area of interest. The hybrid luminaires that delivered the integrated light were composed of modified commercially available fluorescent light fixtures to accept the fiber optic solar light source. The inception luminaires consisted of two light emitting fibers placed strategically inside a traditional fluorescent light fixture, but furthering developments made use of a single light emitting fiber placed in a shallow, space saving design. The new design used a single 3M LF180EXN D side emitting fiber and a system of stranded fibers that utilized the remaining ambient light to the fullest extent. Testing was conducted in the ORNL Illumination Test Cell using a Radiant Imaging Pro-Metric Camera to measure the amount of light reflected off a removable wall coated in Spectralon reflective paint. Efficiency was determined by the totaling up the amount of flux measured off each side of the removable wall. Test results have shown promising results for our new design. The spatial intensity distribution results were less than desirable, but the optical efficiency indicated considerable improvement. The initial goal of the new design was to maximize the efficiency of the natural light, but our research has led to more optimistic anticipation of progressive designs.

Research on Analysis of Integral Pressurizer Design in support of Nuclear Energy Research Initiative (NERI) Project. HORACIO VELAZQUEZ (*Texas A&M- Kingsville, Kingsville, TX 78363*) GRAYDON L. YODER JR., PH.D., P.E. (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The International Reactor Innovative and Secure (IRIS) reactor is a new, pressurized water-cooled nuclear power reactor design. The reactor coolant system design incorporates a pressurizer, steam generators and eight reactor coolant pumps, all contained inside the reactor pressure vessel. The coolant system and its pressurization system are the main components used to improve efficiency and safety over existing reactor designs. Two potential Integrated Primary System Reactor (IPSR) pressurizer designs are being analyzed for this research project: a steam pressurizer, and a nitrogen gas pressurizer. These two integral pressurizer designs differ from most conventional types, because they incorporate a much larger interface more closely coupled to the reactor primary system. In the steam pressurizer design, the large interface between the saturated pressurizer and the subcooled primary coolant may lead to significant heat losses from the pressurizer and require a larger heater power to compensate. In the nitrogen gas pressurizer system, nitrogen diffusion from the pressurizer into the primary coolant can lead to significant quantities of dissolved nitrogen. Some postulated accidents have the potential to release this nitrogen as gaseous bubbles that could negatively impact heat transfer in the core. Engineering calculations examining heat transfer, mass transfer and diffusion

coefficients are being evaluated in order to determine the operational specifications to avoid these negative impacts. In addition to analytical calculations, a computational fluid dynamics model (CFD) of certain parts of the reactor, using the FLUENT code, will be created to determine the operational characteristics of the reactor. These calculations will combine thermal fluid and mass transport to produce an accurate simulation of the reactor system. The ongoing research in this project will combine the analytical calculations and CFD modeling techniques, implemented by the FaST team, to help understand details of the pressurizer operation.

Ring Injection Dump Thermal Transient Analysis. JASON REAGAN (*Pellissippi State Technical Community College, Knoxville, TN 37933-0990*) MARK WENDEL (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The Ring Injection Dump (RID) is part of the Spallation Neutron Source used as a place to stop stray hydrogen atoms that were not captured into the Accumulator Ring. The kinetic energy of these particles is deposited as heat in the RID. A recent steady-state thermal analysis model built in CFX5 has shown that at 200 kW, the bulk temperature of the concrete structure of the RID will exceed 65 °C in some areas, with localized points reaching 91 °C. This violates the upper limit specifications for concrete used in nuclear safety related structures. For this reason, a transient analysis of the RID was performed to characterize the response time to load changes and to verify the amount of load credit taken in the steady-state model to account for system shutdown periods. A new, less detailed model was created with HEATING 7.3. It was calibrated so that its maximum concrete temperatures agreed with the more detailed CFX5 model. The transient was then run for a twenty year simulation, with an assumed ten week duty cycle and an annual shutdown period of ten weeks. The analysis revealed an overall time constant of more than one year. Because the peak temperature in the final years of the transient agreed with the steady-state model, the load credit used in steady-state analysis was verified.

Robotics CAD Modeling: Using SolidWorks™ Software. DARREN NORRIS (*Roane State Community College, Harriman, TN 37748*) CRAIG BRADLEY (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The Remote Systems Group at Oak Ridge National Laboratory is preparing a conceptual design of the remote handling equipment system for a new nuclear waste treatment facility. Because of the high levels of radioactivity expected in the treatment facility, the process components must be maintained and operated remotely. These design efforts are to develop: design requirements for the remote handling equipment, design concepts for the equipment, a maintenance plan, and a cost estimate for the remote handling system. Designing this equipment will help to shape the Archimedes Filter Plant for Archimedes Technology Group, LLC, a private company in San Diego. One of the deliverables for this project is to develop 3-D solid models of the remote handling equipment. This involved learning to use the state-of-the-art 3-D Computer Aided Design (CAD) software, Solid Works™, to prepare the 3-D models of the robotic and remote handling equipment. These models will help engineers design and plan the layout of the robotics equipment going into the Archimedes waste processing facility.

Spectroscopic Exploration of Spark Plug Erosion. KATHERINE WOODY (*Middle Tennessee State University, Murfreesboro, TN 37132*) JOHN WHEALTON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

When voltage is sent to a spark plug in an engine, the voltage causes a spark in the gap at the end of the spark plug. When this spark occurs there is erosion at the site of the spark. Spark plug erosion is caused by several factors, including the material of the spark plug and the pressure of the surrounding gas. This erosion is studied by spectroscopic analysis of the light emitted by the sparks. Through study of sparks in several gases, including argon, nitrogen, and instrument air, it was possible to determine whether a certain line in the spectrum was caused by an interaction with the surrounding gas or gases or by the impact with the electrode. This allows for more direct quantification of erosion per spark. Certain new types of spark plug, particularly a Rotating Arc Sparkplug (RASP), are thought to cause less erosion than traditional spark plugs, as they more evenly distribute sparks across the electrodes. Also, there are continuing studies on the RASP dealing with design and erosion.

Spectrum Analysis of a Spark Plug. CARL ENG (*State University of New York at Stony Brook, Stony Brook, NY 11794*) JOHN H. WHEALTON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The photon emissions generated by the arc on a spark plug may be useful indicators of the materials that are being ablated off the spark

plug. In theory, identifying the wavelengths of light emitted by the excited electrons in the spark plug material as it is being ionized within the spark plug gap would give information on the erosion of the spark plug. Specifically, the magnitude and rate of erosion could be determined on a spark-to-spark basis. Furthermore, the intensity of the spectra from the arc may reveal the ignition capabilities of the arc as some of the observed spectra are believed to characterize the energy of the ionized gas contained in the volume of the spark plug gap. Using a test chamber to vary pressure, spark plugs were run. The light from the spark was focused (via a fiber optic cable and lenses) into a spectrometer. Images of the spectra were then transferred to a computer by a charge injection device (CID) camera. Initial experiments were run on spark plugs designed for operation in a natural gas engine, which focused on a band of wavelengths ranging from 300nm to 750nm. In that range, two distinct peaks at 392.22nm and 395.69nm were observed on the used spark plugs that were not seen on the new spark plugs. Work is ongoing to identify the observed spectra. In addition, experiments are being conducted to establish a correlation between the other observed spectra and possible gas transition states within the arc. An examination of a larger spectrum range is being undertaken with the employment of spectrometers with sensitivities in the ultraviolet and infrared ranges of the electromagnetic spectrum. Initial data has yielded results worthy of further analysis.

Telomere and Chromosome Segmentation and Editing Tool. JUAN AGUILAR (*Richard J. Daley College, Chicago, IL 60652*) TOM KARNOWSKI / KEN TOBIN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The Image Science & Machine Vision (ISMV) Group performs Applied Computer Vision Research & Development to address areas of biomedical, industrial and national security. The goal of this project is to develop a software tool to analyze cellular images in a biological imaging environment. The main development environment used in this project was Microsoft Visual Basic 6.0. The Telomere and Chromosome Segmentation and Editing Tool performs a set of complex algorithms and generates computational graphical data, in order to analyze images to locate the chromosome and telomeres, and estimate its volume. The data collected can successfully be saved and opened in graphical displays in the program. The ISMV Group scientists successfully tested many aspects of the program and reported several bugs as well as initiated new features for the software. The Telomere and Chromosome Segmentation and Editing Tool will provide valuable information to a wide range of biological researchers. The Tool will be used to study the chromosomes. This information is important because it will be used to help determine why people develop cancer.

Test for Disruptions in ControlNet Communications Due to Electromagnetic Interference. COLIN FINUCANE (*University of Kentucky, Lexington, KY 40502*) PAUL WRIGHT (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

ControlNet is a system that enables programmable logic controllers to communicate over RG-58 coaxial cable. Allen-Bradley ControlNet systems are being used in many controls applications at the SNS. It is necessary to ensure that ControlNet systems are capable of communicating in the presence of Electromagnetic Interference. A major source of EMI at the SNS will be the pulsed power sources for the RF Systems. These pulsed power sources known as High Voltage Converter-Modulators utilize relatively new technology. The effects they will have on ControlNet systems using RG-58 media had not been studied. Tests were conducted with ControlNet in which the cable was arranged to maximize the effects from Converter-Modulator produced EMI. Communications were monitored over the network with counters on ControlNet software, counters in the controller's program, and with an oscilloscope for EMI influences on the signal. The tests were performed for the same period of time with the Converter-Modulator both off and pulsing at 120 kV. The results with the Converter-Modulator running did not vary significantly from those with it off. No bad information was received at either end of the RG-58. These results were expected because the ControlNet system is designed to be resistant to EMI. The results indicate that there will be no problem with properly installed systems. The actual systems will have more nodes communicating on their ControlNet networks in the presence of additional Converter-Modulators pulsing at 140kV. Further tests should be conducted with the actual systems when they are installed.

Testing on Op-amps. DERRICK GREEN (*Georgia Institute of Technology, Atlanta, GA 30332*) CHUCK BRITTON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Op-amps are used in almost all electronics presently. However, many op-amps do not perform exactly as they are needed to. Therefore, many times the electronic devices which require their use are not always as

accurate as they need to be. The op-amp under test was specifically designed to have as little as possible of the input-offset error encountered by most op-amps. In order to run the series of tests that were needed to have conclusive results, the computer program Visual Basic was needed. The computer software told the voltage input device when and by how much to increase the voltage and also where to start and begin. Essentially, the input device was controlled remotely from a computer to do the specialized things which this series of tests required. The testing involved running voltages through five different op-amps labeled D2, D4, E3, E4, and E5 at different temperatures. The voltage ranged from zero to 3.3 volts and was increased in increments of 10 millivolts with a 0.2-second delay between each different voltage. At each voltage, five readings were taken with 0.2 seconds in between each reading and then the average was calculated. An offset reading was also taken each day prior to any readings that might be taken. To find the offset, the input voltage was subtracted from the average actual output voltage. Once a sufficient offset was obtained, the input vs. offset data could be calculated. The Agilent 34970A Data Acquisition/Switch Unit was used to control the input voltage and then take the resultant output readings and feed them to the computer software which then put the readings into a spreadsheet in Microsoft Excel. The software did all of the configuring of the 34970A automatically each time. The HP 6236B Triple Output Power Supply supplied voltage to the board. This voltage registered on the Fluke 7911I voltmeter as 3.308 volts DC for most of the readings, but it dropped to 3.307 volts DC for many of the readings at the end, as noted. For the variation of temperature, the Delta 9023 oven was used. The temperature range was from room temperature, which with the door on would range from 32-33°C, to 150°C. Overall, the op-amps tested extremely well. The amount of error was usually no greater than 2 millivolts. Moreover, this error was uniform for the voltages that the chip is supposed to be used for.

Tracking and Monitoring of International Shipping Containers. BENJAMIN HUEY (University of Tennessee, Knoxville, TN 37996) PAUL D. EWING (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The international shipping container industry faces many challenges when transporting goods across the oceans. Due to the large amount of cargo on a ship, only about one in four containers are searched by United States Customs agents for illegal articles when they enter the country. These uninspected containers could potentially contain counterfeit merchandise and pharmaceuticals, illegal drugs, illegal firearms, nuclear, chemical, and biological weapons, or even terrorists who want to bypass immigration. The RF & Microwave Systems Group at the Oak Ridge National Laboratory is working on a solution to give shipping companies better monitoring capabilities of their cargo. A wireless system is being developed that will provide real-time temperature, position, and door seal integrity data from each container to receivers on the ship or at the shipyard. This system will use an advanced radio-frequency spread spectrum algorithm, as well as Code Division Multiple Access (CDMA) and Time Division Multiple Access (TDMA) technologies to allow the system to gather data from a large number of containers. Small scale prototyping and testing have demonstrated that the system is affective at providing position and simulated temperature and door seal data at power levels below 125 mW over a range of about one quarter of a mile in line-of-sight conditions. This was somewhat better than expected by the design team; however the system's performance was not as impressive in a non-line-of-sight environment where one transmitting tag was moved behind a building. Large scale operation will be tested by modeling the system using MatLab™ and Simulink™ software packages. This will allow testing of the spread spectrum and multiple access techniques, while taking into account a wide range multipath losses and interference variables without the investment of producing a large number of prototypes.

Vehicle and Engine Management Prototyping System Wiring Harness. STEPHEN BERNARD (Pellissippi State, Knoxville, TN 37920) SHEAN HUFF (Oak Ridge National Laboratory, Oak Ridge, TN 37831). This project, for the FEERC department, involves designing and build a wiring harness that will connect the Vehicle and Engine Management Prototyping System (VEMPS) Machine up to a Mercedes four cylinder diesel engine. This device controls the Mercedes Engine. The computer in the lab sends directions to the VEMPS in digital signals and the VEMPS then in-turn translates the digital signals into analog signals and relays the information to the Mercedes engine. At the same time the reverse is happening, the VEMPS receives analog sensor signals from the engine and translates them into digital signals to send to the lab computer. Specifically it translates data like engine oil temperature, engine water temperature, crank shaft rotation, cam shaft rotation, The mass air flow sensor (MAF), the fuel rail pressure sensor, engine cool-

ant temperature, intake air temperature etc. In addition to communicating directly with the Mercedes engine, the VEMPS communicates with other controllers, which in turn communicate with the engine. They are the injector drive unit (IDU), and the Throttle control. The IDU is a controller that allows us to tune the fuel injection timing and duration. The throttle controller regulates the intake throttle to maintain engine airflow.

Development of a Laboratory Performance Check Material for the Measurement of Yield Stress Using a Vane Impeller. AMANDA BOLTA (Montana State University - College of Technology, Great Falls, MT 59404) PAUL R. BREDT (Pacific Northwest National Laboratory, Richland, WA 99352).

The vane method is used for measurement of critical yield stress in several fields including nuclear waste treatment, food engineering, soil research, and slurry transport. Currently researchers at the Department of Energy (DOE) Hanford site have used this technique for characterizing nuclear waste slurries. These measurements are currently performed without a reference material with which to test the performance of the instrument and technique of the operator. This can increase the risk of erroneous data collection. The purpose of the research described in this paper is to find a material for performance testing. Using a Haake M5 viscometer fitted with a four bladed shear vane, the yield stress of glass bead samples were measured under several conditions. Although all variables examined (bead size, vane depth, vane size, and rotational rate) had some effect on the yield stress measurement of this particular media type, the immersion depth of the vane during testing was observed to have the greatest effect on the yield stress. In this paper, a data set has been developed that allows the use of glass beads as a material for performance testing with limitations and recommended controls.

Energy Code Compliance in a Detailed Commercial Building Sample: The Effects of Missing Data. RAHUL BIYANI (University of Washington, Seattle, WA 98195) ERIC E. RICHMAN (Pacific Northwest National Laboratory, Richland, WA 99352).

Most commercial buildings in the U.S. are required by State or local jurisdiction to meet energy standards. The enforcement of these standards is not well known and building practice without them on a national scale is also little understood. To provide an understanding of these issues, a database has been developed at PNNL that includes detailed energy related building characteristics of 162 commercial buildings from across the country. For this analysis, the COMcheck™ compliance software (developed at PNNL) was used to assess compliance with energy codes among these buildings. Data from the database for each building provided the program input with percentage energy compliance to the ASHRAE/IESNA Standard 90.1-1999 energy as the output. During the data input process it was discovered that some essential data for showing compliance of the building envelope was missed and defaults had to be developed to provide complete compliance information. This need for defaults for some data inputs raised the question of what the effect on documenting compliance could be due to missing data. To help answer this question a data collection effort was completed to assess potential differences. Using the program Dodge View, as much of the missing envelope data as possible was collected from the building plans and the database input was again run through COMcheck™. The outputs of both compliance runs were compared to see if the missing data would have adversely affected the results. Both of these results provided a percentage compliance of each building in the envelope and lighting categories, showing by how large a percentage each building either met or fell short of the ASHRAE/IESNA Standard 90.1-1999 energy code. The results of the compliance runs showed that 57.7% of the buildings met or exceeded envelope requirements with defaults and that 68% met or exceeded envelope requirements with the actual data. Also, 53.6% of the buildings met or surpassed the lighting requirements in both cases. The dataset of 162 buildings is not large enough to accurately apply these findings to all commercial buildings across the U.S., but it does provide a rough idea of what to generally expect. This database also has other uses such as characterization of commercial buildings by each specific data point and in splitting up the total of 162 buildings into smaller subsets to characterize such groups as large (>5000 sq ft) or small (<5000 sq ft) commercial buildings.

High Voltage Variable Frequency High Q Head. PARIS DELISLE (Blue Mountain Community College, Pendleton, OR 97801) DAVID C. PRIOR (Pacific Northwest National Laboratory, Richland, WA 99352). In the field of mass spectrometry, instrumentation is required that is capable of providing a radio frequency (RF) signal at high voltages for the purpose of converting molecules into ions, or ion fragments, that can then be analyzed with a mass spectrometer. The instrument that performs this function is referred to as a High Q head (HQH), and typically is designed to provide voltages ranging from 500-900 Volts, with a fre-

quency range of 600-800 kHz. For this project, the client has specified an HQH delivering voltages ranging from 500-1500 Volts at frequencies ranging from 50-300 kHz. Due to the broad range of frequencies and voltages required, it was necessary to create an HQH with a 3 position switch for selecting capacitive values, and inductors that are manually interchangeable. Circuit design was simplified using TINA PRO Electronics Lab for Windows. Switching components available in the TINA PRO Parts Library made it convenient to run a succession of circuit analyses, while changing component values after every simulation. This method proved to be very effective for checking predicted circuit responses prior to building the final product.

Measuring the Ionization of the Atmosphere. ERIC RUST (Edmonds Community College, Lynnwood, WA 98036) JEFF GRIFFIN (Pacific Northwest National Laboratory, Richland, WA 99352).

Measuring the ionization of the atmosphere promises to provide individuals with an accurate and cost-effective way to determine the amount of radiation in a surrounding area. We used the charge integration principle in the building and testing of an instrument to measure the amount of ions in the atmosphere. This process involves a 30pF parallel plate capacitor being wired in parallel with a 28pF small area capacitor. A positive DC bias is applied across the circuit to charge the capacitors. After the charging circuit is broken, charged ions entering the parallel plate capacitor cause both capacitors to discharge. To simulate an increase of ions in the atmosphere a Krypton-85 (^{85}Kr) source is placed next to the intake of the parallel plate capacitor. The placement of the ^{85}Kr near the intake of the parallel plate capacitor results in a more rapid discharge of both capacitors. We report on the time constants of the discharging capacitors and how they relate to the conductivity of air. Future work will be done using the air conductivity to determine the exact amount of ions in the region being measured.

Rapid Prototype Production Lab at 2400 Stevens. JOSE RIOS (Washington State University, Richland, WA 99352) GREGORY SPEER (Pacific Northwest National Laboratory, Richland, WA 99352).

In business the goal is to achieve the maximum output at the lowest cost possible. A good example of this goal is the achievements of Henry Ford with Ford Motor Company. In 1909, the Model T was produced by using a new method of production. With the innovation of the assembly line, his vision revolutionized the way mass production of vehicles and products in general are produced (B: Encyclopedia of American History page 1025). This idea of mass production at an efficient rate is what motivated the Electronic Systems Group at 2400 Stevens to create the Rapid Prototype Production Lab (RPPL). The RPPL is dedicated to the production of circuit boards both efficiently and cost effectively. Its efficiency is remarkable. In the time one solder technician can hand produce one complete board, RPPL can produce at an average of 50 boards (depending on the number of components. Figures are based on average times of past project production time). The goal for the Electronic Systems Group was to bring to Pacific Northwest National Laboratory (PNNL) the ability to produce technology in large numbers and in less time saving a project money and man-hours.

Rheological Properties of Generalized Concentrated Suspensions. JAMES KARNESKY (Rensselaer Polytechnic Institute, Troy, NY 12180) FADEL ERIAN (Pacific Northwest National Laboratory, Richland, WA 99352).

The design of systems to affect mobilization, retrieval, and transport of the waste stored in tanks at various DOE sites would be greatly bolstered by an accurate correlation whereby the flow properties may be predicted from a certain basic set of measurements of the solids and liquids involved. To this end, various models were investigated, and it was decided that the most apt description of the phenomenon would be to treat the waste layer as a soft solid, and establish a correlation by which the properties of the waste could be computed as a function of the concentration of suspended particles. Existing correlations were analyzed and tested against experimental measurements of slurries of various properties at a range of concentrations. In addition to this, various methods were tested for the determination of the maximum volume concentration of solids in a given slurry, a quantity needed for models of highly concentrated suspensions. It was found that the best models were those of Guth and Simha or Thomas for relatively dilute suspensions, and that of Frankel and Acrivos for concentrations above about 20% the maximum volume concentration, as determined on the measurement of a slurry which has been mixed and then allowed to completely settle. The data set is small, however, and further analysis is desirable.

The Relationship Between Hydraulic Permeability and Directional Air Permeability in Unsaturated Hanford Sediments. LASHANE CARTER (Eastern Washington University, Cheney, WA 99004) ANDY

WARD (Pacific Northwest National Laboratory, Richland, WA 99352). Models of flow and transport in complex soils require information on hydraulic properties at very small scales. However, this information is difficult to obtain using traditional soil characterization techniques. Air permeability measurements have the potential to overcome this limitation because measurements are rapid and the probe is small enough to allow measurements at very small scales. The purpose of this study to examine the relationship between air permeability, which is easy to measure, and the hydraulic permeability, a required model parameter. A set of vertical and horizontal air permeability measurements were made on a dike outcrop using a portable air permeameter. A corresponding set of vertical hydraulic permeability measurements were made using a mini disk permeameter. Results show a linear relationship between hydraulic permeability and air permeability. Directional air permeability results show that the horizontal permeability is higher than the vertical in fine-textured lenses, with ratios as high as 70:1 (horizontal to vertical). There was very little difference between directions in the coarse-textured soils. These results suggest that that small scale directional air permeability measurements might be useful for predicting hydraulic permeability at similar scales and providing critical input data for numerical models.

Digital Signal Processing for the Ground Fault Monitoring System of the National Spherical Torus and National Compact Stellarator Experiments. JUSTIN PEEL (Idaho State University, Pocatello, ID 83201) HANS SCHNEIDER (Princeton Plasma Physics Laboratory, Princeton, NJ 08543).

The National Spherical Torus Experiment (NSTX) at the Princeton Plasma Physics Laboratory (PPPL) uses an analog-based lock-in amplifier for a ground fault monitoring system. The system is subject to signal phase problems and large amounts of noise. Digital Signal Processing (DSP) techniques were investigated for possible use in upgrading NSTX's Ground Fault Monitor (GFM) and a new system under development for use on the National Compact Stellarator Experiment (NCSX). This investigation involved the development of Finite Impulse Response (FIR) and Moving Average (MA) digital filters and a dual digital lock-in amplifier system in a single DSP board. A system utilizing a DSP board was compared with the existing analog hardware to assess performance and aid in development. The DSP system was found to be somewhat less sensitive due mostly to hardware limitations, but adds phase shift independence and runtime switching of the lowpass filter's time constant.

Phase Noise Measurement in PEP II and the Linac. MESFIN GETANEH (University of New Orleans, New Orleans, LA 70148) RON AKRE (Stanford Linear Accelerator Center, Stanford, CA 94025).

The Goal of this project is to provide a measurement of the phase of the radio frequency (RF) relative to electron beam traveling down the Stanford Linear Accelerator Center (SLAC). Because the Main Drive Line (MDL) supplies the RF drive and phase reference for the entire accelerator system, the phase accuracy and amount of phase noise present in the MDL are very critical to the functionality of the accelerator. Therefore, a Phase Noise Measurement System was built to measure the phase noise in the liner accelerator (Linac) and PEP II. The system was used to determine the stability of the PEP II RF reference system. In this project a low noise Phase Locked Loop system (PLL) was built to measure timing jitter at the sub picoseconds level. The phase noise measured in the Master Oscillator using the PLL system indicates that phase noise is low enough for PEP II to run.

Tuning Broadband Microwave Amplifiers. GABRIEL ALANIZ (Texas A&M University - Kingsville, Kingsville, TX 78363) ANDREW YOUNG (Stanford Linear Accelerator Center, Stanford, CA 94025).

The PEP II DAÖNE/ALS longitudinal feedback systems are complex wide bandwidth systems requiring analog, digital and microwave circuits. The solid-state amplifier is one of the components in the microwave circuit that is required to suppress the coupled bunch instabilities that exist in the PEP-II accelerator. The suppression is achieved by using an antenna as a kicker structure that provides an electric field in order to increase or decrease the energy of particles passing through the structure. The amplifier is made up of sixteen 30 to 35W microstrip GaAs FET modules that are combined to obtain 500W over a bandwidth of 850MHz to 1850MHz. The amplifier malfunctioned causing a reduction in the functionality and power output of the individual GaAs FET modules. The amplifier must be repaired. After repair, the amplifier must be tuned to optimize the gain while maintaining proper power output. The amplifier is tuned using microstrip circuit techniques. A variety of microstrip methods are used to obtain the proper line impedance. The result is a working amplifier that operates efficiently. Work supported by the Department of Energy, contract DE-AC03-76SF00515

Analog Block Testing and Calibration Suitcase. CHARLES PARKER (Bucknell University, Lewisburg, PA 17837) HAI DONG (Thomas Jefferson National Accelerator Facility, Newport News, VA 23606).

At Thomas Jefferson National Accelerator Facility (TJNAF) there is a device in operation called an "Analog Block." An Analog Block is a device that supports a "Trim Card." The Trim Cards are responsible for controlling the current through the electromagnets that guide the electron beam. The Analog Blocks monitor the current through the electromagnets and adjust the output of the Trim Card to compensate for any changes in the magnetic field strength. It is critical that the Analog Blocks be calibrated correctly to ensure that they operate properly. Currently the only method of testing and calibrating Analog Blocks is to remove it from the accelerator and take it to a location that has a large rack of appropriate test equipment. It is desirable to be able to test and calibrate Analog Blocks on location instead of removing it to a nearby facility. A "Testing Suitcase," a self contained testing and calibration device that can be taken onto the accelerator site has been developed. This suitcase is capable of testing both generations of Analog Blocks (I/II). This suitcase should shorten testing and calibration time for Analog Blocks and make them more feasible for use in other applications.

Determining the Modulus of Rupture of Crystal Quartz. JESSICA SHEEHAN (Old Dominion University, Norfolk, VA 23669) KEVIN JORDAN (Thomas Jefferson National Accelerator Facility, Newport News, VA 23606).

Thomas Jefferson National Accelerator Facility Free Electron Laser (FEL), for terahertz (THz) experimentation, is investigating switching to a more economical window made of crystal quartz. Crystal quartz contains the same transmittance qualities as the currently used diamond windows at a fraction of the cost. However, crystal quartz has not been widely used for this purpose. Since the quartz will be in a vacuum, it is pertinent to determine the modulus of rupture of the window, the maximum amount of stress a material can withstand. In order to create creditable data, the crystal quartz had to be characterized through atomic force microscopy, an interferometer, and scratch dig. In addition, a device was created to hold the window (35mm diameter X 2.5mm thickness) in place so that air pressure could be applied in order to discover the modulus of rupture. This is particularly important since transmittance is an exponential function related to thickness. If a window would transmit 10% at some thickness, but since the modulus of rupture is unknown the window is made twice as thick for safety reasons, it would now only transmit 1%. Three crystal quartz windows were tested, which resulted in the discovery that the majority of the literature is incorrect in suggesting the weakness of the material. The windows held to 250psi, without any visible damage. Since the modulus of rupture was not actually determined, thinner windows were ordered to continue the experiment. These windows also held to 250psi without visible signs of damage, which had led to a design change in the testing chamber to allow more area to be tested.

Isolation for Maintenance of Helium-Refrigeration Systems. TERESA BONK (Binghamton University, Binghamton, NY 13902) DANA ARENIUS (Thomas Jefferson National Accelerator Facility, Newport News, VA 23606).

Until recently TJNAF's Cryogenics Systems Group relied on the manufacturer's manuals when conducting maintenance activities on the helium-refrigeration systems. In May 2003, TJNAF's management declared that the manufacturer's manuals were not sufficient. Management further delegated to the group the task of developing and documenting procedures for isolating and disconnecting specific subsystem equipment. First, a general familiarization of the cryogenics system processes and their operational and maintenance requirements had to be achieved. Next, identification of subsystems that require isolation for maintenance, while maintaining continuous plant operation, needed to be established. Then, the operations of each of the major subsystems and the hazards that need to be isolated and controlled during maintenance were recognized. These subsystems include helium gas compressors, cold box housing, turbo-expanders, gas storage, and gas purification equipment. Finally, procedural documentation, that instructs maintenance personnel how to isolate and control the hazards, was developed for some of the above equipment. The procedural documentation was submitted for formal review and approval to the Cryogenics Systems Group Leader. The results are 'Equipment Specific Personal Safety Lockout/Tagout (LOTO) Procedures' for maintenance of nine different systems. These procedures will be utilized for maintenance activities on these cryogenic systems once personnel have been trained.

ENVIRONMENTAL SCIENCE

A Perspective on Current Computer Models and Codes for Use in Site Decontamination. VICTOR CORDOVA (University of Illinois at Chicago, Chicago, IL 60612) BRUCE M. BIWER (Argonne National Laboratory, Argonne, IL 60439).

Radioactively contaminated sites can be dangerous areas for anything or anyone nearby. Cleanup of these sites depend on the types of radionuclides or contaminants present. Environmental scientists attempt to estimate the threat presented by the contaminant dose. Previous investigations and experiments have assisted computer models in generating their own dose and risk estimates. Models such as Residual Radioactive (RESRAD), Generation II-Version 2 (GENII 2) and others, attempt to provide reasonable approximations on the risk to humans. Documents such as reports and manuals are available as forms of assistance in becoming acclimated with the programs. These documents contain parameter information, measurement methodologies, exposure pathways, and explanations on how the programs estimate dose and risk. Discrepancies amongst the models occur because of their intended use, which might cause users to question their reliability. Often, the models contain similar parameters, but differ in wording and/or methods of measurement and distributions. Currently, the Cleanup Sub-Committee of the Interagency Steering Committee on Radiation Standards (ISCORS) is in the process of providing an on-line catalog of environmental parameter information sources, acting as a single repository of information for use by the various models.

Analysis of Trace Metal Complexation with Carbonate Species in Lake Pleasant, Pennsylvania. SUZANNE QUARTUCCIO (University of Virginia, Charlottesville, VA 22903) DAVID S. MILLER (Argonne National Laboratory, Argonne, IL 60439).

Lake Pleasant is an archetypical glacial lake community which supports a wide diversity of organisms including several species of special concern. The Western Pennsylvania Conservancy and the Environmental Assessment Division (EAD) of Argonne National Laboratory are monitoring current conditions in the lake and accessing changes to minimize adverse effects. Elevated trace metal (Cd, Cu, Pb, Hg and Zn) concentrations have been measured in surface water, groundwater and sediment samples collected from Lake Pleasant in 1991-2002. This study investigated the possible explanation of trace metal complexation with carbonate species for the reduced toxicity of the elevated metal concentrations. A better understanding of the interactions between metals and the carbonate system will help maintain the integrity of the lake. Evidence for complexation was based on past research studies of lakes with similar conditions as Lake Pleasant with respect to pH, alkalinity and hardness. Stability constants were also used in this study to ascertain which species predominate under certain conditions. The results show that the carbonate system of Lake Pleasant does effectively form strong complexes with copper and lead. Weaker carbonate complexes are formed with cadmium and zinc. Mercury does not complex with carbonate to a significant extent but does form strong hydroxide complexes. Carbonate complexation reduces the toxicity of the metals to species by reducing the availability to be assimilated. Hardness ions, correlated with carbonate, also reduce toxicity as calcium and magnesium compete with trace metals for binding locations on plants and animals. Based on the findings presented in this study, elevated trace metal concentrations do not pose a risk to the species of special concern in Lake Pleasant as long as the carbonate and correlated hardness systems remain intact. To ensure the quality of the lake, the Western Pennsylvania Conservancy and EAD should continue monitoring carbonate and metal concentrations every summer.

Assessing the Risk to Populations Exposed to Radionuclide Contamination: Creating a Database to Make Relevant Data more Accessible. ERICA EMMY (Augustana College, Rock Island, IL 61201) BRUCE BIWER (Argonne National Laboratory, Argonne, IL 60439).

When an area of land or a building is contaminated by radionuclides, it is necessary to assess the threat posed on a person's safety. The population can be exposed to radiation through both internal and external pathways, and to determine the risk which a person faces from these pathways, values for specific parameters need to be known. In order for potentially hazardous areas to be assessed, computer programs based on mathematical models were created, which professionals used to perform risk analyses. However, separate government agencies were in charge of oversight in different areas, and each agency created their own computer model to meet its needs. The models, although very similar, were different, and as a result the assessments performed by different agencies on the same problem were not always in agreement. Thus the need to standardize radionuclide contamination assessment was

realized, and the Cleanup Sub-Committee of the Interagency Steering Committee On Radiation Standards (ISCORS) sponsored the creation of a web-site database as one step to accomplish that goal. The aim of the web-site is to provide information and relevant references regarding parameters considered in four models: RESRAD (RESidual RADio-activity), EPA-PRGs (Environmental Protection Agency Preliminary Remediation Goals), GENII 2 (Generation II, Version 2), and DandD (Decontamination and Decommissioning). The recommended sources for parameter data will enable professionals to spend less time searching for good information and more time making informed assessments.

Changes in the Vegetation Cover in a Constructed Wetland at Argonne National Laboratory, Illinois. COURTNEY BERGMAN (*Olivet Nazarene University, Bourbonnais, IL 60914*) KIRK LAGORY (*Argonne National Laboratory, Argonne, IL 60439*).

Wetlands are valuable resources that are disappearing at an alarming rate. Land development has resulted in the destruction of wetlands for approximately 200 years. To combat this destruction, the federal government passed legislation that requires no net loss of wetlands. The United States Army Corps of Engineers (USACE) is responsible for regulating wetland disturbances. In 1991, the USACE determined that the construction of the Advanced Photon Source (APS) at Argonne National Laboratory would damage three wetlands. Argonne National Laboratory was required to create a wetland of equal acreage to replace the damaged wetlands. For the first five years after this wetland was created (1992-1996), the quality was closely monitored. The wetland was not monitored again until 2002. In 2003, the vegetation cover data was again collected. The plant species were sampled using quadrats at randomly selected locations along randomly selected transects throughout the wetland. The fifty sampling locations were monitored once throughout the summer and percent cover of each of the plant species was determined for each plot. Furthermore, the water cover in the wetland was measured. In 2003, 21 species of plants were found and identified, and four species were found but not identified. The grasses found were not identified or separated by species. Eleven species dominated the wetland, among which were reed canary grass (*Phalaris arundinacea*), crown vetch (*Coronilla varia*), and Canada thistle (*Cirsium arvense*) all non-native species. In the previous year, 30 species were found in the same wetland. The dominant species varied from the 2002 study but still had these non-native species in common. Unfortunately, these non-native species may be contributing to the loss of biodiversity in the wetland. In the future, control measures should be taken to ensure the establishment of more desired native species.

Communication of Health Risk Information from Chemical Releases in Buildings. MIRIAM KIM (*UIC, Chicago, IL 60645*) MARGARET MACDONELL (*Argonne National Laboratory, Argonne, IL 60439*).

Chemicals that are released in buildings can cause substantial amount of concern and damage when preparedness and the communication of risk information is inadequate. Collaborating with the U.S. Environmental Protection Agency (EPA), the U.S. Department of Energy Chicago Operations Office (DOE CH)-Argonne National Laboratory (ANL) recently initiated a rapid risk assessment program to support the EPA National Homeland Security Research Center, with buildings as the primary focus. In the midst of emergency conditions varied messages may be given to the public due to the multiple agencies involved who may have different information specific to them and may use different communication methods. Providing information and technical resources for building security, emergency preparedness, first responders, and the general public is crucial for protection, improved decisions, and effectiveness of response measures. The nature of this study is to review existing agency resources and other literature and determine key inconsistencies or gaps to identify where information can be improved. Information relevant to risk communication concerning buildings and hazardous chemical releases was evaluated and similarities and differences among agencies were identified. One recommendation is to develop fact sheets for specific target audiences within the general public, including teachers and students, to help address potential health concerns. The duration of the new EPA-ANL project is anticipated to continue for three years in order to provide emergency responders and the public with the necessary information and tools to ensure maximum safety and protection for all citizens.

Development of a Wastewater Land Application Permit Application for the Industrial Waste Pond at Argonne National Laboratory-West. ERIK AKINS (*Idaho State University, Pocatello, ID 83209*) TIM MILLER (*Argonne National Laboratory, Argonne, IL 60439*).

The Industrial Waste Pond at Argonne National Laboratory-West currently needs a Wastewater Land Application Permit. This permit is issued by the Idaho Department of Environmental Quality after the characteristics of the pond have been reviewed. Three pieces of information

need to be collected for the permit application: the current water level and when the pond is projected to go dry, the flow of the water into the pond, and the levels of specific constituents. There are four parts to this internship and they are; to research the requirements for a wastewater land application unit, compile the information required for an application, draft an application, and track/monitor the water level for the IWP to determine when the pond will go dry.

Development of Zinc-Extraction Procedures from Mint and Marigold Plants for Use in Phytoremediation Studies for Middle and High School Levels. JAMES LEE (*University of Illinois at Chicago, Chicago, IL 60612*) DEON ETTINGER (*Argonne National Laboratory, Argonne, IL 60439*).

The process of phytoremediation through the use of plants is an inexpensive and environmental friendly method for cleaning up heavy metals at toxic levels in the environment. An objective of the project at Argonne National Laboratory was to confirm the uptake of zinc into the leaves, stems, or shoots of marigold and mint plants. The second objective was to develop a safe and simple zinc-extraction procedure that allows middle and high school students to carry out experiments in the classroom, in order to study the process of phytoremediation. Marigold and mint plants displayed a significant uptake of zinc in plant leaves and stems after watering for four weeks with 1 ppt zinc nitrate solution three times per week. The uptake of zinc in the plant leaves, stems, and shoots from concentrated soil was analyzed using X-ray fluorescence. The extraction procedures for recovering the zinc from plant cells involved drying the plant samples, grinding the samples into a fine powder, washing in diluted HCL acid solution, and filtering with Whatman #1 filter paper. The result for zinc extraction from 1.15 g of mint plants was 0.451 ppm and from .73 g of marigold plants was 0.309 ppm. When students submit their plant samples to ANL, DEP personnel will analyze solid samples for zinc using X-ray fluorescence and the extract of zinc from plant cells using flame atomic absorption spectroscopy. The research indicated that marigold and mint plants would be good choices for analyzing the uptake of zinc in plants and that the process of phytoremediation can be studied in the classroom by using these adapted zinc-extraction techniques.

Emissions Inventory for Air Pollutants in the Las Vegas Valley. HETAL PATEL (*Loyola University, Chicago, IL 60625*) MICHAEL LAZARO (*Argonne National Laboratory, Argonne, IL 60439*).

Air pollutants which are released into the atmosphere through various sources have been harming the environment and humans as well. The air pollutants are of special concern in the areas that do not meet the standards set forth by the Environmental Protection Agency (EPA). Although, the Las Vegas Valley is a nonattainment area for particulate matter (PM10) and carbon monoxide, other pollutants, namely sulfur dioxide, volatile organic compounds, and nitrogen oxides, were also studied. Four different source categories, precisely stationary point, stationary area, on-road mobile and non-road mobile, were studied in order to obtain accurate data. The data for the sources had been collected for 1998, which were used to extrapolate emissions for 2000, a base year for this study. Data for stationary area and non-road mobile sources as well as the results from a micro-scale inventory of the five ambient sites are included. The emission factors were all published in AP-42 on the EPA website. The activity levels were extrapolated using 1998 data from the PM10 State Implementation Plan developed by Clark County. Most of the activity levels depended upon the change in population, therefore a growth factor of 1.100 was predicted from 1998 to 2000 and the activity levels were modified accordingly. The actual emissions were then calculated using the emission factors and activity levels of each source. The data has been organized into a spreadsheet, which will be used to create a Geographic Information System (GIS) – based model. Results are in preliminary stages as the project is still in progress. The Bureau of Land Management (BLM) manages the public land in the Las Vegas Valley and is expected to increase the rate at which the disposals occur, which has heightened public concern of air resources. Hence, Argonne National Laboratory was entrusted with the task of modeling the air quality to support the BLM's plans for land disposal and maintain a healthy and safe environment.

Monitoring the vegetation characteristics of Wetland R of Argonne National Laboratory-East, Illinois. JAMARIS EALY (*University of Illinois-Chicago, Chicago, IL 60651*) KIRK LAGORY (*Argonne National Laboratory, Argonne, IL 60439*).

The construction of the Advanced Photon Source building at Argonne National Laboratory caused the destruction of Wetlands A, B, and D. Wetland R was a mitigation wetland established in August, 1991, to replace these destroyed wetlands. By taking the topsoil of the destroyed wetlands, the species were moved to Wetland R. Methods of sampling vegetation involved the collecting and pressing of species. For each

species found, a sample was taken and photographed as an aid for species identification. Photographs taken with a digital camera and other tools were used for data collection. The progression of the growing of vegetation was evident when focusing on the increased percent cover of the dominant species. With much of the invasive species decreasing in percent cover, the wetland has more space to grow other species since the 1996 data collection. In conclusion, the usage of different technological tools (digital camera, computers) enables data collection to be more time efficient and have less experimental error. The usage of these tools can also open doors for other areas of research within the project.

Identifying Potential Problem Areas in the Design and Filtration of Local Exhaust Ventilation Systems at Brookhaven National Laboratory. TRACY JACKSON (Tulane University, New Orleans, LA 70118) JOHN PETERS (Brookhaven National Laboratory, Upton, NY 11973). It is very important to the workers safety, the working environment, and the atmosphere that local exhaust ventilation (LEV) systems, used for the capture of hazardous materials and vapors, have correctly designed stacks and adequately maintained High Efficiency Particle Absolute (HEPA) filters if they are needed. The purpose of this project was to evaluate the LEV systems of buildings to determine if the correct design criteria are met, and to update the information and database regarding HEPA filters. It is a pilot study to develop the inspection criteria, practical documentation methods, and determine the time and resources needed for project completion. Conducting a questionnaire with administrative and technical personnel as well as taking guided tours of the interior and exterior of the buildings was the method of data collection. It was found that 43% of the stacks on the roof of Building 480 are mushroom caps, which do not meet the height requirement, and there is a stack releasing carcinogenic and nitrate vapors very near an air intake. Building 463 has a HEPA filter that is only performing at 85% efficiency when 99.97% is desired. Also, all of the surveyed stacks on the roof of Building 463 are made of galvanized steel, which is prone to rusting and developing holes. It is recommended that the mushroom stacks at Building 480 be replaced with stacks meeting the height requirement, and that the stack located near the air intake either be decommissioned or redesigned. The HEPA filter for lab 264 at Building 463 should be evaluated for correct installment and filter type, and the life cycle costs for the galvanized steel stacks should be assessed to see if replacement is feasible. Not only was this valuable information found but also the procedure for surveying the LEV systems in a building was developed and can be used on the remaining buildings at Brookhaven National Laboratory.

Mapping Invasive Species of Long Island. TIM WALTERS (SUNY ESF, Syracuse, NY 13210) PETER KELLY (Brookhaven National Laboratory, Upton, NY 11973).

Invasive plant species have been an issue of concern on Long Island for many years whose spread has become an issue of increasing concern due to their displacement of naturally occurring plants and natural habitat composition. In order to establish effective methods of eliminating/controlling these species on Long Island requires information pertaining to introduction into an area, rate of spread and likely vehicle(s) of transmission between areas is needed. Initial infestation data was collected and map overlays were developed using GPS and ArcMap/View software. In doing this, shape-files were created in three forms (point, line, polygon) depending on dimensional characteristics of infestations ensuring accuracy of data collected. Visual aides (map overlays) were then created allowing the comparison between previously undisturbed areas with disturbed areas that now serve as habitat for invasive plants. These weed occurrences were also imported into a database (along with additional field data collected) that may be made the standard for all noxious/invasive weed occurrences nationwide that will allow the sharing of information pertaining to them including effective control measures. As may have been expected, there was a direct correlation between where these developments took place and the currently infested areas. It could also be seen that areas likely to receive the highest frequency of disturbance by people/vehicles, seemed to have a higher amount of (in some cases more dense) occurrences. This project will serve as a foundation for future comparisons and will serve as the initial data that will be used to compare changes in size, density, and numbers of occurrences in the years to come.

Material Inventory Analysis in Manufacturing $\text{Cu}(\text{In}_{0.75}\text{Ga}_{0.25})\text{Se}_2$ Photovoltaics. DANIEL CHERN (Columbia University, New York, NY 10027) VASILIS FTHENAKIS (Brookhaven National Laboratory, Upton, NY 11973).

Potential environmental effects of producing the materials used in manufacturing $\text{Cu}(\text{In}_{0.75}\text{Ga}_{0.25})\text{Se}_2$ (CIGS) photovoltaic cells are examined. Information is gathered concerning the mining, extraction, and purification

or the three metals, which are used in these cells: indium, gallium, and selenium. Most of the information was collected from Kirk-Othmer Encyclopedia of Chemical Technology and Ullmann's Encyclopedia of Industrial Chemistry. Other major sources were the USGS: Mineral Commodity Summaries of 2002, US Patent Office, and Andersson's Material Constraints on Technology Evolution. The information was compiled to describe various mining, extraction, and purification processes and some emissions and waste streams. Indium comes from zinc ore, which undergoes flash roasting or fluidized roasting, and then is leached and purified by electrolysis or cementation. Gallium primarily comes from bauxite ore by means of the Bayer process, extracted by the Beja, de la Breteque, Rhône-Poulenc, or Sumitomo processes, and purified by electrolysis, filtering and heating, gradual crystallization, or conversion to halides. Selenium is separated from copper ore in copper smelters as electrolytic copper refinery slimes, extracted by roasting in soda or sodium carbonate, Outokumpu Oy Process, or wet chlorination, and then purified by vacuum distillation or vaporization. This paper is a compilation of information needed for the initial step for a complete report on the life cycle analysis of the CIGS photovoltaic cell.

Photovoltaic Installation Environmental Health & Safety Issues.

KIM TRAN (University of South Alabama, Mobile, AL 36695) VASILIS FTHENAKIS (Brookhaven National Laboratory, Upton, NY 11973). This project studies the risks related to PV installation and maintenance. In the analysis of environmental, health, and safety (EHS) concerns associated with photovoltaic (PV) systems, two issues that will be discussed are risk of fall from the roof by installers and electrical hazards to repair personnel. The homeowner as well as the system installation or repair personnel should be aware of the risks associated with photovoltaic systems so that unnecessary injuries may be prevented. Rooftop installations are of particular concern due to the risk of injury associated with climbing on and off the roof as well as while working on the roof. Since there are no statistics that characterize installation of PV systems, the roofing industry is used here as a reference. The Bureau of Labor Statistics was used as the primary source for data to develop rates for both fatal and nonfatal injuries and illnesses among all workers, construction workers, and roofers specifically. Analysis of the statistics on injury and fatalities shows that the risk of injury to roofers, both fatal and nonfatal, is one and a half times higher than those in general construction. One area of concern in installation and maintenance of PV systems is electrical shock to individuals performing work on the PV modules or those who inadvertently come into contact with components of the PV systems. The maximum peak current produced by modules used in residential buildings ranges from approximately 3A to 7A; this level of current is enough to cause nerve damage and muscular contractions. Three situations in which the potential for electrical shock may occur will be discussed in this document: open lines from the inverter, islanding, and improper grounding

Qualitative Investigation and Identification of Odonate Larvae at Brookhaven National Laboratory. SUSAN COSTA (Community College of Rhode Island, Warwick, RI 02886) TIMOTHY M. GREEN (Brookhaven National Laboratory, Upton, NY 11973).

The Order Odonata is believed to have appeared about 250 to 300 million years ago during the Carboniferous period, which was part of the Paleozoic Era. Based on fossil records dragonflies of this time period were huge with wingspans that measured up to 70 cm (27.5 in.). Over time they have diverged into two Suborders, Zygoptera (damselflies) and Anisoptera (dragonflies). The purpose for conducting the research at Brookhaven National Laboratory (BNL) was to identify and catalog the specimens found at the laboratory. The goal was to identify the specimens down to the species level whenever possible, and to compare the distribution of the various species across all ponds studied. Some of the ponds selected for the research have historically been used by the tiger salamander (*Ambystoma t. tigrinum*) and are designated as P-1, P-2, P-6, P-7, P-9, and P-10 (P standing for pond). Several of the ponds near the Relativistic Heavy Ion Collider (RHIC) were also sampled. One of the ponds is referred to as the "9 O'clock Pond" and the others are referred to as Recharge Ponds A6a, A6b, A6c and A6d. The Peconic River was also sampled specifically for Ebony Jewelwing larvae because it is the only location on the Lab where the adults have been found. Once a pond was selected, a dip net, seining net, or a minnow trap was used to collect specimens out in the field. Specimens were temporarily stored in Ziploc bags and placed in a cooler on ice. The purpose for the ice was to keep specimens alive and immobile while identifying them in the lab. Once specimens were brought into the lab, a dissecting microscope and taxonomic keys were used to identify specimens to genus and species. By project end, seven dragonfly larvae have been identified to the species level, two have been identified to the genus level and three damselflies have been identified to the spe-

cies level. Anisoptera larvae identified at BNL include *Anax junius* found at P-10 and 9 O'clock Pond, and Recharge Basins A6a, A6b, A6c and A6d; *Aeshna umbrosa* found at A6d and the Peconic River; *Anax ion-gipes* found at P-7, *Somatochlora williamsoni* found at P-10, *Symphtrum janeae* and *Pachydiplax longipennis* found at P-1, *Libellula semifasciata* found at P-7; and *Dythemis sp.* found at P-2 and P-7, but could not be identified to the species level. Zygoptera identified at BNL were: *Enallagma durum* found at P-10, *Lestes eurinus* found at P-1, and *Lestes unguiculatus* were found at P-2 and P-1. Future research may expand to other ponds as part of a larger on going biotic inventory of the lab.

Site Testing at a Coal-Fired Power Plant for Mercury Deposition. GENEANE WALSH (*The Richard Stockton College of New Jersey, Pomona, NJ 08240*) BIAYS BOWERMAN (*Brookhaven National Laboratory, Upton, NY 11973*).

The purpose of this project is to collect and analyze samples to characterize mercury deposition trends around a coal-fired electric power plant. Several studies of mercury deposition have shown that both wet and dry deposition transfer airborne mercury to the terrestrial environment. Therefore, mercury concentrations in soil around the power plant will provide an integrated deposition history and can be used to judge the impacts of the power plant on deposition. Modeling of mercury deposition from power plants suggests that wet deposition due to scavenging of mercury by rain drops will lead to deposition rates on the order of background or greater in a small almost circular region 5 - 10 km around the plant. Dry deposition peaks further from the plant in the direction of the prevailing wind. Vegetation and soil will be collected at selected sites within 25 kilometers coal-fired power plant. Integrated mercury concentration in air will be determined using the moss bag technique. All the samples are taken back to the lab for analysis using the Milestone Direct Mercury Analyzer (DMA). The analysis time for each sample is 6 minutes using the DMA. To provide a baseline for the method, soil and vegetation samples from BNL were collected in June from 2 locations: the softball fields and the field between the Guest House and Brookhaven Center. The initial results from the samples collected at Brookhaven National Laboratory showed more variability than expected. The DMA was blowing some sample particles out of the boats; this caused the sample weight to be lower than the weight entered and therefore gave high results. There were also system malfunctions due to the ambient lab temperature. In order to address these problems, the DMA was to be moved to another lab. Results from soil samples collected on site show that the maintenance of the DMA helped to improve the samples were more measurement precision. GIS maps are being created for several candidate sites. Within the next few months, samples will be collected from at least one Power Plant site. Future plans for the experiment are to collect samples from a number of different Power Plants in the United States.

Culex Mosquitoes at Fermilab and West Nile Virus. CHRISTINE BRAYER (*University of Illinois at Chicago, Chicago, IL 60612*) ROD WALTON (*Fermi National Accelerator Laboratory, Batavia, IL 60510*). The most common vector of West Nile virus in Illinois is the mosquito *Culex pipiens*. *Culex pipiens* feed mainly on the blood of birds, but are known to bite a variety of animals including humans. In 2002, Illinois lead the country having the greatest number of human, West Nile virus cases. Increasing incidences of West Nile virus have been associated with decreasing bird populations in the areas surrounding Fermilab. Fermilab's bird counts have gone up in recent years, indicating that West Nile virus is not present on Fermilab grounds. Eight Fermilab sites with characteristics conducive to the breeding of *Culex pipiens*, and one site lacking those characteristics, are tested for the presence of the mosquito using stagnant-water Gravid trap. The trap is designed to capture female *Culex* mosquitoes when depositing their eggs after having a blood meal. Captured *Culex* mosquitoes are tested for West Nile virus using a rapid immunochromatographic assay that will detect the protein antigen found in the gut of a mosquito that has fed on a host carrying the virus. Variations in the mosquito populations among the sites are found which are attributable to both ecological and human-induced (e.g., pesticide spraying) factors. Over 900 *Culex* mosquitoes are captured and more than 500 are tested for West Nile virus. All tests are negative, which may account for the increase in Fermilab's bird population in contrast to the surrounding area.

Grassland Birds at Fermi National Accelerator Laboratory: A Study of Bird Populations, With Respect to Vegetation Density and Plant Species Diversity. SHANNON MURPHY (*University of Illinois at Chicago, Chicago, IL 60607*) ROD WALTON (*Fermi National Accelerator Laboratory, Batavia, IL 60510*).

Nationwide, grassland bird species have declined, due to habitat loss, inadequate land management and habitat fragmentation. Fermi National Accelerator Laboratory (Fermilab) of Batavia, Illinois has

dedicated over 1,000 acres of land to reconstruction of natural grassland. Studying six sites on Fermilab property this study estimated the population of three grassland specialists and the Red-winged Blackbird because of its abundance. In order to determine if there was a correlation between bird populations and site characteristics such as plant density and diversity and land management practices. Timed transect studies were performed to gather bird population data. Robel measurements and primary plant species diversity was recorded to provide site characteristics. Multiple Regression analysis was used to assess the impact of vegetation on bird abundance for each species on the independent variables (Robel Scores and diversity measures). T-tests were used to determine whether bird population estimates are different in burned sites versus mowed sites. The results of the analysis showed no correlation between bird population and plant characteristics. The results did demonstrate a negative correlation between Red-Winged Blackbird abundance and the target species, which suggests further research to explore whether blackbirds exclude others or other species do not prefer the same habitat as blackbirds. The data suggests Savannah Sparrows and the three target species together prefer unburned mowed sites. Further research may be conducted to determine species preference for burned versus mowed sites and the land management implications.

Preventing Noncompliance: Tank Evaluations. LAURA THOMPSON (*Tennessee Technological University, Cookeville, TN 38505*) RHONDA OSBORNE (*Idaho National Engineering & Environmental Laboratory, Idaho Falls, ID 83415*).

Every producer of waste is faced with the challenges of protecting the environment and maintaining environmental compliance. U.S. Department of Energy National Laboratories are no exception to this rule. Faced with this responsibility, the Idaho National Engineering and Environmental Laboratory (INEEL) has developed a program to verify and update tank information, thus fulfilling their environmental policy. The program determines what tanks need to be evaluated and provides the means for the evaluation. Tanks selected for the program are validated and updated by interviews, documents, physical inspection, and sample analysis. Research about the tank history and generation process is conducted. The responsible party is verified and contacted. Data are collected to determine the exact location via global positioning system (GPS) technology. Photographs and measurements are taken to accurately describe the tank. Tank contents are evaluated to determine if they are product or waste. Finally, if needed, a hazardous waste determination is performed per Resource Conservation and Recovery Act (RCRA) regulations or follow-on actions are identified. The tank information is updated in the database and all supporting documentation is recorded. As this process continues, regulatory conflicts are addressed and the potential for noncompliance is reduced. Although the program is not complete, some results can be evaluated. The program has shown the importance of communication within the laboratory. While every department shares the common goal of preventing noncompliance, they do not all speak the same language. The program has, also revealed the importance of maintaining the database to reflect changes in tank status, location, contents, etc. The program will conclude when all tanks have been verified and any identified follow-on actions have been addressed. The result of these activities will be more accurate tank information thereby reducing the potential for noncompliance.

Application of remote sensing in measuring and monitoring wetland habitat. SARA FELDMANN (*California State University Hayward, Hayward, CA 94542*) NIGEL QUINN (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Remote sensing is providing new opportunities for the development of wetland best management practices in California's central valley. High-resolution satellite imagery is available in five spectral bands that can be digitally blended into a high contrast composite. This composite image forms the basis for new research in measuring and monitoring wetland habitat in Grasslands Water District (GWD). GWD supplies water to approximately 50,000 acres of seasonal wetlands in the San Joaquin basin. The wetlands are intensively managed for wintering waterfowl and migratory shorebirds by manipulating flooding and drainage schedules, irrigation, as well as methods for controlling undesirable vegetation. Wetlands are subject to Basin Plan water quality objectives that limit salt load discharges to the San Joaquin River, so best management practices need to meet the dual objectives of enhancing wetland function and meeting river water quality objectives. Remote sensing will allow for development of a wetland model that includes water quality and flow data, as well as detailed information relating changes in vegetation to management practices. Initial habitat mapping is currently underway using IKONOS satellite imagery with 4-meter resolution in red, blue, green and near-infrared bands and 1-meter resolution in

panchromatic. Composite images are then georeferenced using field surveys and GPS data, and will ultimately provide a key for interpreting unique wavelength signatures. Preliminary research indicates that remote sensing can effectively isolate individual plant communities for quantification. Refinement of these techniques will provide wetland managers with information to improve water use efficiency and enhance wetland productivity.

Calibration of a Portable Sampler for Environmental Tobacco Smoke. MAISHA MURRY (*Tuskegee University, Tuskegee, AL 36088*) MICHAL APTE (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

A portable sampler for environmental tobacco smoke (ETS) is being developed to assess the potential misclassification of acute ETS exposure status changes over short periods of time. A simple, inexpensive portable sampler is being designed for sampling ETS particle matter (PM), nicotine, and 3-ethenyl pyridine (3-EP). A series of chamber experiments were performed to calibrate the prototype portable sampler. We found that the thermophoretic particle sampler (TPS) component is collecting ETS adequately and that the amount of ETS collected can be deduced from the absorbance of ultraviolet light by the ETS deposit on the TPS. By comparing UV absorbance and other instrument's measurements of ETS concentration we were able to calibrate the TPS response to ETS. More chamber experiments are needed to validate its specificity for ETS.

Comparative Fatty Acid Methyl Ester Analysis of Fungi. MARIA JIMENEZ (*Austin Community College, Austin, Tx 78751*) TAMAS TOROK (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*). Microorganisms living under extreme environmental conditions, such as high temperature, and a wide range of pH, salinity and radiation have been most often the target of bioprospecting efforts. Forty-one filamentous fungal isolates from several geothermal sites in Kamchatka, Russia and radiation contaminated environment in Chernobyl, Ukraine were subjected to fatty acid methyl ester (FAME) analysis to explore their degree of relatedness. Understanding their taxonomic and functional diversity supports a better understanding of biogeothermal processes in the environment and may provide clues for discovering new biochemicals or capabilities for commercialization. Data collection required a highly standardized process of culturing, lipid extraction, fatty acid methylation, and the quantitative analysis of FAME's using a gas chromatograph equipped with a flame ionization detector (FID). Major peaks were further analyzed with Sherlock² software and plotted as dendrograms, histograms, and 2-D principal component diagrams. FAME dendrograms use statistically assigned numbers - Euclidian distance - that cluster related chromatograms based on pair-wise fatty acid comparisons. Among the 35 Kamchatka and 6 Chernobyl isolates there were seven and three cultures respectively that showed significant taxonomic differences to warrant attention for further biochemical studies. Isolates that show distinct taxonomic properties often display more interesting physiological attributes for bioprospecting.

Electronic Control System for Prototype Laser Ultrasonic sensor. HAMIDREZA HAMEDTOOLLOEI (*Contra Costa College, San Pablo, CA 94806*) PAUL RIDGWAY (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

Ultrasonic plate waves can be employed to measure the elastic properties of paper without touching it. A pulsed laser generates the ultrasonic wave. The wave travels along the sheet, and is detected at a known distance by an interferometer. The time of flight of the wave over the known distance gives the propagation speed of the wave, which is related to physical properties of paper. This system works well for stationary paper. It would be useful to measure elastic properties of paper on the papermaking machine as the paper moves at manufacturing speeds up to 30m/s. However, some modification is required for moving paper because the surface roughness of moving paper creates signal noise unless the detection beam is moved with the paper so that the detection point does not change location on the paper surface for the duration of a measurement. The detection beam is moved by deflection from rotating mirror. As the mirror spins, the beam is reflected in a circular pattern. During a portion of each revolution, the beam meets the paper, and remains on the same detection point throughout its brief contact with paper since both the beam and the paper are moving at the same speed. The generation laser is triggered at the proper moment by a computer-controlled timing system.

Implementation of Particle Monitoring Instrumentation for Particulate Matter Exposure Assessment. MIGUEL CHARLES (*University of Texas at Brownsville, Brownsville, TX 78521*) MICHAEL (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

A major limitation of current methods for particulate matter (PM) expo-

sure assessment methods is their inability to simultaneously assess multiple characteristics of PM. This limitation makes environmental tobacco smoke (ETS) characterization subject to misclassification bias. Other limitations of PM exposure assessment technology include the high costs, size, weight, noise, and power constraints. This study focuses on developing portable, cost-effective exposure assessment devices capable of integrating different exposure assessment technologies to improve PM characterization. These devices implement optical particle characterization by measuring the absorbance of light from the ultraviolet (UV) to near infrared (NIR) spectrum. Particle collection on sampling surfaces is accomplished by thermophoresis (TP). My work has focused on the design of the electronic control circuitry and instrument packaging for the Tobacco Related Disease Research Program (TRDRP) device, as well as conducting chamber experiments and collecting and analyzing experimental data to evaluate the performance of ETS assessment devices. To address the portability and cost sensitive issues, a peripheral interface controller (PIC) was designed and evaluated to control and log data allowing for freestanding sampling. Implementation of a real time clock and temperature sensor for real time and temperature data acquisition was approached using 1 wire technology provided by Dallas Semiconductor. The passive gas sampler incorporates stepper motor control and infrared optical sensing to collect one-week integrated samples. The final design will be embedded in a camping lantern shell and deployed to field to monitor ETS exposure.

Importance of Phosphate to Algal Biomass Growth in Agricultural Drainage. ERIC AMARO (*Miami Dade Community College, Miami, FL 33014*) WILLIAM STRINGFELLOW (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

Introduction Large amounts of algae in the San Joaquin River attribute to the dissolved oxygen deficit. My project this summer involved finding a relationship between concentrations of Chlorophyll-a (used to measure quantity of algal biomass) and ortho-phosphate (o-PO₄). Another purpose of my analysis was to show correlations between amount of o-PO₄ and inorganic suspended solids. The hypothesis is that o-PO₄ is a limiting nutrient of algal growth and found in agricultural drainage. Method Analysis of o-PO₄ was according to Standard Method 4500-P C, the Vanadomolybdophosphoric Acid Colorimetric Method. Chlorophyll a analysis was according to Standard Method 10200 H, by spectrophotometer determination. The analysis of suspended solids was according to Standard Method 2550. Results were measured using a Perkin Elmer UV/VIS Double beam Spectrophotographer. Results The concentration of chlorophyll a increases as the water flows down the San Luis Drain and reaches maximum growth by mile 15. In contrast, concentration of soluble o-PO₄ continues to decline over the entire length of the drain. The concentration of o-PO₄ in the drain is closely correlated with the concentration of suspended mineral solids. Conclusion Concentration of o-PO₄ decreases as the amount of algae biomass increases over the length of the drain. The relationship between algal growth and o-PO₄ concentration is not conclusive, but ortho-phosphate cannot be ruled out as a potential limiting nutrient. Inorganic suspended solids are closely correlated with o-PO₄ concentrations, indicating that the removal of suspended solids would be an important step in achieving o-PO₄ control in this system.

Integration of Optical Analysis into New Particle Collection Devices. PATRICIA CLORE (*University of Kentucky, Lexington, KY 40502*) MICHAEL G. APTE (*Lawrence Berkeley National Laboratory, Berkley, CA 94720*).

For the past decade, understanding the link between particulate matter (PM) exposure and human health has been at the top of the U.S. environmental agenda. Exploring this link requires a more accurate description of exposure than is available with the current instrumentation. Of the devices currently available to monitor PM exposure, none are capable of simultaneously assessing multiple PM mass and chemical characteristics. Development of the next generation of PM detectors aims to incorporate monitoring of PM mass, size and composition simultaneously. This study focuses on composition determination. Diesel exhaust, environment tobacco smoke (ETS), and wood smoke are three of the most abundant species of PM. LBNL researchers have found that the differing optical properties of each enable speciation. Previous experiments show ETS strongly absorbs ultraviolet wavelengths. Black inorganic carbon aerosols, such as diesel exhaust, absorb equally at all wavelengths. Other PM species display characteristic spectral absorption ratios. In controlled chamber experiments, we have studied optical reflectance attenuation due to absorbance of ETS, collected using a novel particle collection system. With the use of Ocean Optic's light source and spectrometer, the full spectrum of reflected light can be compared with incident light. Absorbance measurements are being integrated into two novel particle detectors for both real-time and

post-collection analysis. These characterization efforts and the future characterization of other PM species are crucial for the development of an internal miniaturized optical system for portable PM instrumentation.

Life Cycle Cost and National Energy Savings Analysis for Residential Furnaces and Boilers. WEIHUA ZHANG (*Laney College, Oakland, CA 94607*) ALEX LEKOV (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Life Cycle Cost (LCC) and National Energy Savings (NES) analysis are part of a comprehensive impact analysis for a new energy efficiency standard for residential furnaces and boilers. The objective of LCC analysis is to demonstrate cost the consumers pay over a furnace or a boiler's lifetime, and purpose of NES analysis is to estimate monetary savings from natural gas and electricity use at different energy efficiency levels. We perform LCC and NES analysis to six furnace and boiler product classes. They are non-weatherized gas furnace, weatherized gas furnace, manufactured-home gas furnace, oil furnace, oil boiler, and gas boiler. Using Monte Carlo simulation method to account variability, we randomly sample data from 2,876 households selected by Energy Information Administration (EIA)'s 1997 Residential Energy Consumption Survey for each simulation. The Crystal Ball program performs a total of 10,000 simulations for each efficiency level with design improvement. The data are extracted to MS Excel spreadsheet, and their mean values are documented in summary files, and DOE will consider these summary results as factors for selecting the new standard in the final rulemaking in 2004.

Predicting Cell Wall Surface Layer in Bacilli Strains. CRISTINA RAMIREZ (*Austin Community College, Austin, TX 78751*) MARTINE SEVIK AND TAMAS TOROK (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Some eubacteria are enveloped in a paracrystalline protein structure known as the surface layer or S-layer. Each strain makes a unique protein. S-layers have properties that can be exploited. These properties are in vivo or in vitro self-assembly of a regular lattice, where 30%-70% of the lattice consists of pores. The S-layers can be modified by covalently binding functional groups for the development of vaccines, or antibodies for immunoassay dipsticks (Sleytr 2000). Because S-layers form a regular lattice on a nanometer scale, they may be developed for semiconductor and nanotechnology (Sleytr 2000). Using these proteins in industrial processes may expose them to extremes in temperature, pH, and pressure. An elegant solution is to collect bacterial strains that are adapted to extreme environments. The current method of proving a strain has an S-layer is through electron microscopy (EM). This technique is time consuming, labor intensive, and costly. Our project is to develop a practical method for ranking a group of unknown strains according to the likelihood that they produce S-layers. The strategy is to use simple, rapid methods that alone prove nothing, but that taken together, allow ranking the strains. There are certain criteria that can be used as guidelines. Messner (1984) reports that the S-layers of Bacilli are usually a prominent band on a gel, and fall between 80 and 160 kDa. S-layer protein makes up 5-10% of the total cell protein. Several methods can be used in such a strategy. These are whole cell chemical extractions, extraction through limited enzymatic degradation of the cell wall, repeated subculturing, and amplification of the SLH, a non-unique region of homology. Two of these methods were used to collect circumstantial evidence, whole cell chemical extractions and repeated subculturing. At this point in the project, including protease inhibitors will be evaluated to ascertain if they must be included to optimize the system. Cell lysis is a problem with *B. amyloliquefaciens*. Sorbitol was added to extraction buffers to maintain the osmotic balance. It has been observed that cells subjected to subculturing lose their S-layers (Sleytr, 1999). This phenomenon can be exploited to collect evidence of an S-layer. Since S-layer proteins make up 5-10% of all cellular proteins, the disappearance or fading of a strong band in the MW range of 80-160 kDa would provide circumstantial evidence for S-layer existence.

Retro-Commissioning of Educational Buildings for energy savings. JIANQING REN (*Laney College, Oakland, CA 94607*) PHILIP HAVES (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

This project is to re-commission educational buildings in Oakland. Retro-Commissioning is a process to ensure the design, installation, functionality, operation and maintenance of the existing buildings. Retro-Commissioning can reduce operation costs, maintenance costs and improve the comfort for the occupants in the existing buildings and extend the life of equipment. This project involves with Quantum Energy Services and Technologies Inc., city of Oakland, and LBNL. The project began in June, 2003. The project commissioned 11 buildings at Laney College campus and 9 buildings at Merritt College campus. A survey of HVAC system, mechanical system, electrical system, and indoor comfort are conducted at Laney College and Merritt College. Numbers

of problems have been found. The major problems are non-working economizer dampers, dirty filters, dirty cooling and heating coils, low efficiency equipments, and poor fan maintenance. Excess lighting exists in libraries, classrooms and offices. After analyzing the survey and collected data, we found that lighting adjustment has the biggest energy saving potential. Lighting controls and energy saving sensors need to be installed. Delamping the offices, classrooms and libraries will reduce the electricity usage. Replacing fan motor belts, changing filters regularly and setting up a good control schedule will decrease usages of gas and electricity. The annual energy saving will exceed to several thousands of dollars.

Using the Terrarium as a Model Ecosystem to Teach Grammar School Students About Their Own Ecosystem. SHANNA CASPI (*Lesley University, Cambridge, MA 02138*) KATHY BARRETT (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Many times students fail to make the connection between what is taught in the classroom to the reality outside. With the fierce reality of environmental hazards, teachers need to use the classroom experiences to increase knowledge and heighten awareness to the needs of the environment. Observation of a number of hands-on summer science camps and participation in a teacher workshop shows the usefulness of hands-on science activities and science inquiry in doing scientific investigations. Additional readings, such as *The Teaching of Science in Primary Schools*, focuses on efficient questioning strategies and conducting strong student-focused investigations. Combining all the information provides insight to the fact that using real-life models in the classroom does increase science content, but further extensions must be made in order to make the connections to the outside world. Creating an extension to the GEMS curriculum *Terrarium Habitat* < Kimi Hosoume and Jacqueline Barber, 1994> allows students to use the terrarium as a model ecosystem in order to investigate the ecosystem of their school and their personal surroundings. Using the initial observations, students gather information and skills that prove to be useful as they further investigate the characteristics of the school's ecosystem. With a student-centered model for teaching, based on ideals of science inquiry, students see that their lives are directly connected with the natural world around them, an important component in environmental awareness and action.

Application of Pyrolysis Molecular Beam Mass Spectrometry (py-MBMS) to Agricultural Soils from the Conservation Reserve Program in the Historic Grassland Soils of the United States.

GABE OLCHEIN (*Colorado State University, Fort Collins, CO 80521*) KIM MAGRINI (*National Renewable Energy Laboratory, Golden, CO 89401*). Applying rapid throughput pyrolysis molecular beam mass spectrometry (py-MBMS) to soil samples enables soil organic matter (SOM) components to be both quantified and chemically identified. SOM formation and dynamics is a complex process that includes the transformation of organic material into more stable humic substances through microbial action and/or chemical degradation. Well-characterized soil samples from a multi-state study of native, cropped, and Conservation Reserve Program (CRP) soils were selected for this study. This sample set is unique because it has been extensively characterized for physical and chemical properties and allows us to measure how well py-MBMS can chemically characterize SOM. For this work, we used a subset of these well-characterized soils, which had not been analyzed by mass spectrometry, to further explore the application of py-MBMS analysis as a way to predict SOM characteristics currently obtainable by chemically damaging, time-consuming, and expensive conventional techniques. Preliminary statistical observations revealed the relationships between SOM characteristics and various management practices the soils had been exposed to under CRP, indicating which practices were best at adding carbon to the soils. Multivariate analysis, including projection to latent structures (PLS) modeling, demonstrated that py-MBMS could be used to predict the percent soil organic carbon in soil with a high correlation and predictability, 95 and 94%, respectively. Further modeling may identify other SOM characteristics that can be predicted by our py-MBMS technique. These include, but are not limited to: Delta C13, soil microbial biomass, total soil N, inorganic particulate matter, particulate organic matter, and mineral-associated carbon.

Assessing the Cost and Benefits of Instream Flow Mitigation at Hydroelectric Plants. BRIAN HATTON (*Ball State University, Muncie, IN 47306*) MARK BEVELHIMER (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Hydroelectric projects alter the natural flow regimes of streams. License articles that govern project operation often include flow regulations in an attempt to minimize environmental impacts. These mitigative measures come at an expense to the power companies. The objective in this study was to evaluate the environmental benefits of increased flows

relative to economic costs (i.e., generation and facility improvements). Projects that had a recent change in instream flow requirements were identified and then stream flow and fish monitoring data downstream of the project were obtained. Daily mean stream flow data for the past several years was gathered from the United States Geological Survey's (USGS) website. Using the "Indicators of Hydrologic Alteration" (IHA) software, an analysis was done on stream flows before and after flow regulations were changed. Changes in operations were detectable for several of the IHA parameters, such as monthly, weekly, and daily minimum flows. Finding biological data was more difficult, thus making the benefits of flow improvements more problematic to assess. Data from previous studies on fish and invertebrates were found for some projects. Economic data was found for projects involved in a mitigation study conducted by the Department of Energy. It was concluded that the costs of setting minimum flows is significant, but in the few cases of biological monitoring that were found, the environmental benefits were significant as well.

Assessing the Potential Impact on Drinking Water Sources from Urban and Agricultural Pesticide Applications. ALISON GOSS (*Purdue University, West Lafayette, IN 47907*) 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 are largely unaccounted for. The US EPA estimates nearly 70 million pounds of pesticides are applied to urban lawns each year. This figure does not include pesticides applied to non-residential areas such as golf courses, landscaping around municipal buildings, parks, and other maintained areas in urban watersheds, collectively known as urban and recreational grasses. 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 potential impact of urban-applied pesticides. A rating scheme was developed to identify watersheds with high potential for drinking water contamination by urban-applied pesticides. The degree and characteristics of agricultural-pesticide application in those watersheds identified as having a high potential for drinking water contamination was examined in order to determine the levels of regulated contaminants under National Primary Drinking Water Regulations (NPDWRs). 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. A significant number of urban watersheds were found to have a high potential for impact, and the spatial visualization of these points provides a means of focus for mitigating urban impact to drinking water quality.

Development and Modification of Geosoft Executables to Process Magnetometer Readings for Better Detection and Characterization of Unexploded Ordnance. SIDNEY HALE (*University of Tennessee at Chattanooga, Chattanooga, TN 37403*) THOMAS J. GAMEY (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The inherent inability of magnetometers to distinguish individual magnetic sources has led to the need for a plethora of filtering algorithms to be developed and implemented in the Geophysical Software Package OasisMontaj developed by Geosoft Inc. Most of the new or modified algorithms implemented in OasisMontaj were designed by Thomas J. Gamey and needed implementing in GXC, or Geosoft Executable Code. Some of these algorithms were originally developed in FORTRAN by Thomas J. Gamey and colleagues. The incorporation of FORTRAN code presents a major issue, since there exists no direct implementation of FORTRAN in OasisMontaj. The FORTRAN code must then be converted to C in order to link properly with a GX, or Geosoft Executable. This conversion can be achieved by using a program called F2C, or FORTRAN to C. The C code that is produced by this conversion may sometimes be unusable, since the conversion is imperfect. This imperfection in the conversion process can lead to advanced error accumulation in the data being processed. There is, however, a second method for implementing these FORTRAN functions in a GX. The GNU GCC, or GNU's Not UNIX GNU Compiler Collection, can link objects of various languages together. Thus forming a coherent dynamic-link library, DLL, from the FORTRAN routines and the C wrapper functions needed to allow access to the Geosoft function libraries. These libraries are essential for performing various operations on the dataset contained in the OasisMontaj database as well as for allowing the DLL to produce direct output. Therefore, library integration is an essential issue to

Thomas J. Gamey's research project, An Advanced Magnetic System for High-Resolution Mapping of which this project is a subset. This project is therefore essential to the expeditious filtering of large datasets for the purpose of mapping the whereabouts of unexploded ordnance in a field setting. Student's Name: Sidney I. Hale II School Student Attends: University of Tennessee at Chattanooga Name of Mentor: Thomas J. Gamey Division: ESD Program: DOE SULI

Effects of Antibiotics on the Responses of Fish Embryos to Toxicants. MARI CARTER (*Knoxville College, Knoxville, TN 37921*) MARK GREELEY (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Antibiotics are occasionally used in toxicity testing to distinguish between the effects of bacterial contamination and the chemical toxicants being tested. Recent studies in this laboratory have suggested that antibiotics may affect the results of chemical toxicity tests through a mechanism other than disease prevention and control. The objective of these studies was to determine whether the use of antibiotics in test media alters the responses of test organisms to reference toxicants including potassium chloride (KCl) and copper chloride (CuCl₂). Embryos of the medaka (*Oryzias latipes*), a small Japanese fish widely used for biomedical studies and toxicity testing, were exposed to varying dosages of KCl and CuCl₂ in the presence or absence of a penicillin and streptomycin mixture. Embryos exposed to both toxicants in the presence of antibiotics had higher LC50s (the concentration of a chemical toxicant that causes the death of 50% of the test organisms) than embryos exposed to the toxicants in the absence of antibiotics. These results indicate that antibiotics included in test media can alter the dose-response curves of chemical toxicity tests involving medaka embryos. Other preliminary evidence in this laboratory indicates that antibiotics can also alter the dose-response curves of newly hatched fish (fry). The mechanism(s) by which antibiotics affect the responses of fish embryos and fry to toxicant exposure remain under investigation. Student's Name: Mari Carter School Student Attends: Knoxville College Name(s) of Mentor(s): M.S. Greeley Division: Environmental Sciences Division Program: Pre-Service Teacher Program

Estimating Carbon Sequestration Rates According to Regional Climate and Changes in Land Management. BROOKE CHICHAKLY (*Tulane University, New Orleans, LA 70118*) TRIS WEST (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Carbon sequestration in soils has been identified as a possible method for partially mitigating greenhouse gas emissions. Rates of carbon sequestration vary between land management practices and climate regimes. Quantifying the rates and duration of carbon sequestration under different land management practices is necessary for use in climate change mitigation policy and analyses of national carbon budgets. In order to quantify rates of carbon sequestration per land management practice in each climate regime, a climate classification system was developed based on a combination of the Holdridge Lifezone classification and a more simplified classification introduced by the Intergovernmental Panel on Climate Change (IPCC). Soil carbon data were compiled from experiments that considered changes in soil carbon with changes in management on agricultural lands and grasslands/pastures. Data were aggregated with respect to land management and climate region. Combining all data across land management and climate regions, agricultural lands can sequester 55 g C m⁻² yr⁻¹ and grasslands can sequester 31 g C m⁻² yr⁻¹. These estimates reflect only changes in management within existing ecosystems, and do not represent changes in land cover (i.e., conversion of agriculture to grassland). Agricultural lands may sequester more soil carbon in moist climate regions than in dry regions, while grasslands may sequester more soil carbon in warm climates than in cold climates. Land management practices within climate regions, resulting from this research, are expected to provide more accurate representations of regional sequestration potential and be of use in policy frameworks that monitor carbon sequestration.

Flush of Carbon Dioxide from Rewetted Soils: Comparisons of Different Forest Ecosystems. DEANNE BRICE (*University of Tennessee, Knoxville, TN 37996*) CHUCK GARTEN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The flush of carbon dioxide that results from wetting dried soils has been proposed as a relatively simple method for evaluating soil microbial activity and carbon mineralization. The objective of this study was to examine the flush of carbon dioxide following the rewetting of dried soils from various forest ecosystems. Soil cores were collected in the spring 2001 from three different forest sites on the Oak Ridge Reservation and at four sites in the Great Smoky Mountains National Park. In the laboratory, simple physical methods (wet sieving) were used to separate soil carbon into particulate organic matter and mineral-associated organic matter at these same study sites. The mineral soil from the various sites was sieved using a 6.3 mm mesh sieve and dried at room

temperature (22°C). Twenty grams of the dried soil were placed in an incubation jar and re-wetted to field capacity. Gas samples were taken from the headspace of each jar at 24, 48, and 72 hours after rewetting. Carbon dioxide concentrations were measured using a Hewlett Packard Series II 5890 Gas Chromatograph. The flush of CO₂ was normalized for the amount of soil carbon residing in particulate organic matter (i.e., the portion of soil that is readily available for decomposition by heterotrophic soil microorganisms). For many soils, the concentrations of CO₂ increased rapidly and attained a steady state after three days. Valley soils showed higher production of CO₂ than soils from ridges and slopes on the Oak Ridge Reservation indicating a higher level of soil microbial activity and more soil carbon mineralization. High elevation soils (1430 to 1570 m) from the Great Smoky Mountains National Park exhibited higher CO₂ production than soils from low elevations (530 to 560 m). The trend for both sets of comparisons was increasing CO₂ production from warm, xeric sites to cool, mesic sites suggesting that soil moisture and not temperature was controlling forest soil microbial activity at the time of soil sampling. This method has been previously applied to agricultural soils and also appears to be appropriate for the rapid estimation of microbial activity in forest soils.

Fly Ash Leaching and Carbon Sequestration. ROSHITHA DUNSTAN (Washington University, St. Louis, MO 63130) ANTHONY PALUMBO (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Carbon sequestration in degraded lands has become of great interest. Low pH and poor moisture retention capabilities are often characteristic of these areas. This project examines the impact of the use of fly ash (a by-product of coal combustion) and biosolids as amendments to these lands. The goal of the amendments is to reclaim the lands and to enhance carbon sequestration to compensate for continued use of coal. The fly ash raises soil pH, increases moisture retention, and supplies base cations. In the field it has increased carbon content in the soil. Biosolids act as promoters of organic matter establishment within the soils. However, leaching of metals from the amendments is an important concern. Mixtures of these amendments were created and applied to soils to determine the potential for leaching of metals from the amendments. Samples were run in two time courses. One assay was allowed to incubate overnight while the other assay was allowed to incubate for two weeks. Leaching tests were conducted using leaching columns and calcium chloride and the effluent was analyzed by inductive coupled plasma mass spectroscopy (ICP-MS). Other tests performed included nitric acid extractions and hot water boron extractions. In addition, tests for cation exchange capacity, electric conductivity, and heavy metals were conducted on the different amendments. The results will help indicate if the amendments will be feasible on a large scale.

Global Climate Change and Forest Tree Distribution: Does Acclimation Play a Role in the Response of *Betula alleghaniensis* to Warming? SUSANNA HUTTON (Spelman College, Atlanta, GA 30314) CARLA A. GUNDERSON (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

It is predicted that rising levels of CO₂ in the atmosphere will cause global warming, possibly resulting in a change in the distribution of many forest tree species. By the year 2100, it is estimated that air temperature will rise an average of 1 - 4.5°C. In 2002, research began to study growth and photosynthetic acclimation of three species of forest trees in response to simulated climate changes. Nine open top chambers (OTC) were built outside to provide warming treatments for two species of trees native to Tennessee and further south, and one species, *Betula alleghaniensis*, native to northern regions of North America. Although *Betula alleghaniensis* is found in generally cool regions, it is possible that it could acclimate to increased temperatures produced in the OTC. It is hypothesized that *Betula alleghaniensis* will adversely react to increased temperature. Unlike the two native species, *Betula alleghaniensis* may show reduced growth in warmer temperatures and fail to fully acclimate in the southern portion of its current range. In order to simulate a change in global climate, OTC are maintained at ambient temperatures, ambient + 2.5°C, and ambient + 5.0°C. Responses, including growth, phenology, and physiology, are monitored throughout the year. Using a portable photosynthesis system, data is collected by measuring photosynthetic rates at temperatures 21°C- 39°C. Rates were logged every 3°C. A parabolic equation fit to each temperature response curve was used to calculate the optimum temperature for photosynthesis in each treatment and the photosynthetic rate at that temperature. Curves reveal species acclimation, and may also show adverse affects to increased temperatures. Results showed that *Betula alleghaniensis* did not positively adjust to increased growing temperatures. The optimum temperature for photosynthesis in *Betula alleghaniensis* did increase by 2°C in warmer chambers, but photosynthetic rate decreased about 13% from ambient chambers to ambient + 5°C

chambers. Although *Betula alleghaniensis* may show some acclimation in terms of optimum temperature, it reacted adversely in terms of photosynthetic rate. Temperature optimum for *Betula Alleghaniensis* did not significantly increase with warming. Seedlings were apparently unable to fully acclimate. It is not clear whether this species will disappear from the warmer parts of its range in the future.

Oxidation-Reduction Reactions Influencing Cr(VI) Transport in Hanford and Ringold Formation Sediments. ROYCE SPARKS (Berea College, Berea, KY 40404) MELANIE MAYES (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Cr(VI) is a major contaminant below the leaking underground waste storage tanks at the DOE's Hanford, WA., Reservation, and has been found in the ground water below the tank farms as well as in the nearby Columbia River. The migration of Cr(VI) is generally promoted in negatively charged subsurface sediments because it exists as the anionic species Cr₂O₄²⁻. The goal of this research was to provide a better understanding of the geochemical interactions of Cr(VI) with Hanford and Ringold sediments, which comprise the unsaturated vadose zone beneath the tank farms. This research will lay the groundwork for undisturbed core studies to investigate coupled geochemical and hydrologic processes that contribute to the overall mobility of Cr(VI). Using kinetic batch adsorption experiments, the geochemical interactions of Cr(VI) with the sediments were quantified. Centrifuge tubes were filled with 4 g sediment and 8 ml Cr(VI) (0.2 mM) solution and agitated for various time intervals ranging from seven hours to upwards of thirty days. The solutions were removed from the tubes following centrifugation and analyzed by UV/Visible spectrophotometry for Cr(VI) and Atomic Absorption spectrophotometry for total Cr. There appears to be reactivity causing loss of Cr(VI) in the Hanford sediments, however it did not react with the Ringold sediments. Kinetic rate coefficients were generated for the removal of Cr(VI) from solution, and the reaction was determined to be first-order. It is proposed that Fe(II) sources in the Hanford formations are responsible for the reduction of Cr(VI) to an insoluble and less reactive Cr³⁺ form. Magnetite, ilmenite, olivine, and biotite are possible sources of Fe(II) needed for the reduction reactions. It is likely that such Fe(II) sources have been oxidized to Fe(III) in the older Ringold Formation. A Hanford repacked saturated column was also used to study the interaction of Cr(VI) with the sediment under flowing conditions. Initial result suggest that long time frames (~10 days) are needed to complete the reduction of Cr(VI) to Cr(III) in some Hanford sediments. It is also possible that Cr(VI) reaction is very limited in some Hanford sediments. These results when combined with future undisturbed column studies will lead to a better understanding of the reaction mechanisms and migration of contaminants at the Hanford site.

Patterns in United States Anthropogenic Carbon Emissions on a State-by-State Basis. CHRISTINE BRONIAK (The Pennsylvania State University, University Park, PA 16802) T. J. BLASING (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

State-level fossil fuel carbon emissions estimates were developed using data from the State Energy Data System of the U.S. Department of Energy. Data for 1960-2000 coal, petroleum products, and natural gas were given in heat units. Carbon contents per unit of heat were applied to obtain carbon emissions numbers. Some petroleum products (e.g. petrochemical plastics) are not exposed to oxidation. The percentages of oxidized carbon given by the U.S. Environmental Protection Agency, in various reports, were used to determine carbon oxidized for each petroleum product class. Per capita carbon emissions values were then obtained for each state. The preliminary results show that per capita carbon in California has decreased since 1960 while the per capita carbon values in Wyoming and the four corner states have increased nearly sevenfold since 1960. This could suggest that electricity for California is being produced in those other five states. Coal used for electricity in these states increased from 80,000 billion Btu in 1960 to about 2,800,000 billion Btu in 2000. Population in the four corners states and Wyoming only increased by 275% from 1960-2000. These results indicate increased electricity production in these states for export elsewhere. The results are expected to be useful in developing carbon emissions reduction strategies for the United States.

Photosynthesis Response to Temperature. ANDREW MCFALLS (Roane State Community College, Harriman, TN 37748) CARLA GUNDERSON (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Photosynthetic temperature acclimation is being investigated as part of a larger project of forest response to global warming. The three species involved in this project were Liquidambar styraciflua (sweetgum), *Betula alleghaniensis* (yellow birch), and Quercus rubra (northern red oak). This project focuses on just the *Quercus rubra*. These trees are planted in outdoor chambers known as the "Open top chambers" (OTC). There are nine temperature-controlled chambers in which these trees are

planted. The first temperature treatment uses ambient or normal outside daily temperatures. The next is 2.5°C warmer, with the third temperature being 5°C above ambient. These temperatures are controlled by computers connected to heating/cooling units on each chamber. The project investigates whether the *Quercus rubra* seedlings will acclimate to the warmer temperatures predicted with global warming. A portable photosynthesis system was used to measure leaf photosynthesis at a range of temperatures. Two trees from each chamber were tested for temperature response. The data were used to calculate the temperature optimum (T-opt) and maximum photosynthesis (P-opt). The average T-opt for the ambient treatment was 24.6°C with the P-opt at 9.3 $\mu\text{mol m}^{-2} \text{s}^{-1}$. For the +2.5 seedlings, the T-opt was 31.8°C with P-opt at 9.7 $\mu\text{mol m}^{-2} \text{s}^{-1}$. For the +5 treatment the T-opt was 33.7°C with the P-opt at 10.4 $\mu\text{mol m}^{-2} \text{s}^{-1}$, which indicates both a shift in temperature tolerance and an increase in carbon fixation at all temperatures. These results will be compared with patterns of leaf phenology and seedling growth. The results to date show that *Quercus rubra* may be able to adapt to temperatures 2.5 degrees warmer, but may have trouble surviving if the atmosphere warms by 5°C.

Hybrid Dataset for Developing High-Resolution Models and Empirical Downscaling Methods. JARED FOX (*Arizona State University, Tempe, AZ 85281*) STEVEN GHAN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Assessments of the impacts of climate change typically require information at scales of 10 km or less. In regions with complex terrain, much of the spatial variability in climate (temperature, precipitation, and snow water) occurs on scales down to 10 km or less. Since the typical global climate model simulation's grid size is over 200 km, it is necessary to develop models with much higher resolution. Unfortunately, there are no global datasets currently produced that are both highly accurate and provide data at a sufficiently high resolution. However, there are several datasets that, if combined appropriately, can provide such a global dataset. We have therefore combined those datasets to produce a global hybrid dataset with information for precipitation, temperature, and relative humidity. The resulting dataset illustrated the importance of having high-resolution datasets. The figures give clear demonstration that regions with complex terrain require a fine resolution grid to give an accurate representation of their climatology. For example, the Andes Mountains in Chile cause a temperature shift of over 25°C within the same area as a single 2.5° grid cell from the NCEP dataset. Fortunately the CRU, U.D., GPCP, and NCEP datasets, when hybridized, are able to provide both precision and satisfactory resolution with global coverage. This composite will enable the development of both high-resolution models and quality empirical downscaling methods.

A Method to Evaluate the Canadian Contribution to Pollution in the Northwest. KAREN CRANE (*Seattle Pacific University, Seattle, WA 98119-1997*) CARL BERKOWITZ (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Because air pollution does not recognize international boundaries, there is reason to suspect that air quality in the Pacific Northwest may be influenced by pollution coming south from Canada. To evaluate this possibility, a large field program to study pollutant patterns over southern British Columbia and northern Washington during the summer of 2001 was conducted. As part of this study, PNNL's Gulfstream-1 aircraft made six sampling missions, carrying instruments capable of making gas and aerosol measurements. These measurements included: position, O₃, SO₂, NO, NO_x, HCHO, CPC (7nm, 12nm, 20nm), UCPC, PCASP, and FSSP. Using a program called Igor, graphical tools have been developed to show the results of these measurements. The graphical presentation consisted of plotting circles along the flight path of the G-1 missions and coloring them to represent the magnitude of the pollutants. In addition, a macro was developed to represent the wind speed and direction every sixty seconds along the flight path using arrows. A software package, called HySplit, designed by National Oceanic and Atmospheric Administration (NOAA) to identify the source of pollutants (both aerosol and trace-gases) was also used. HySplit used wind fields measured during the campaign to compute back-trajectories from points of interest. The preliminary results suggest that many of the high pollution measurements were associated with large urban areas within the northwest, rather than transport from Canada into the United States. These results will also be used in the design of a possible future campaign to look more closely at the distribution and physical properties of aerosols in this region.

Assessment of the Reproductive Fitness of Cheatgrass (*Bromus tectorum* L) on the 100B/C Remediation Area on the Hanford Site. RUTH DELAWARE (*Truman State University, Kirksville, MO 63501*) JANELLE DOWNS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

At the Hanford Site in Washington State, the U.S. Department of Energy (DOE) is working to remediate the 100B/C Area's contaminated solid-waste storage areas. After the remediation, DOE will sample and evaluate post-remediation environments to "demonstrate protectiveness" with respect to soils and biota. One aspect being investigated to demonstrate protectiveness is the comparison of plant vigor between remediated sites and reference sites where no contamination existed. Measuring the reproductive fitness of a species is one way to evaluate the health of biota and thus demonstrate protectiveness. We expect there to be no difference in the reproductive fitness of cheatgrass between the remediation sites and reference site if remediation at the 100B/C Area is successful. Measurements of density, height, number of seeds, seed biomass, and vegetative biomass were taken from the samples collected at the remediated and reference sites. Comparisons of these data indicated that the characteristics were highly variable between and within sites. The calculation of the ratios of "seed biomass/vegetative biomass" or "number of seeds/vegetative biomass" standardized the data, so that variation resulting from environmental factors could be limited. An analysis of variance (ANOVA) for groups with unequal replication was calculated so that the sites could be compared. We found that there was no significant differences existed for either "seed biomass/vegetative biomass" or "number of seeds/vegetative biomass" between the sites. The next step of this project is to conduct germination tests using the seeds collected.

Characterization of Columbia River Nearshore Riparian Breeding Bird Populations at Hanford. MARYLEE STRUB (*University of Idaho, Moscow, ID 83843*) COREY DUBERSTEIN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

It is not known which breeding-bird species are present or at what abundances they occur within many of the riparian plant communities along the Columbia River nearshore environment at Hanford; particularly in those areas that pose risk to wildlife from Hanford-derived contamination. During June 2003, a preliminary study was undertaken to provide an inventory of bird species, their abundance and density within previously mapped riparian plant communities along the Columbia River at Hanford. Seventy-two surveys were conducted. A total of 482 individuals representing 36 bird species in 21 families were observed within 18, 100-m fixed-radius survey points. From a total of 28 mapped riparian plant communities 15 were surveyed. Birds were found in 11 out of the 15 surveyed riparian plant communities. Greater than 50 percent of the bird species observed occurred in the Low Shrub-Cobble association. The Wormwood/Perennial Grass association was the second largest in terms of area, however, species richness was low, totaling 3.9 species/ha. Across the survey sites, the most abundant bird species were the red-winged blackbird observed in 5 out of 11 plant associations, and the European starling found in 3 out of the 11 surveyed plant associations. The California quail, eastern kingbird, and yellow-headed blackbird were observed in 5 out of 11 plant associations surveyed.

Dust monitoring on the Hanford Site: An investigation into the relationship between TSP, PM-10, and PM-2.5. TARA SCHWARTZ (*University of Idaho, Moscow, ID 83843*) BRAD FRITZ (*Pacific Northwest National Laboratory, Richland, WA 99352*).

High levels of particulate matter (PM) are linked to some health problems and environmental issues. Air quality standards have been developed in hopes to reduce particulate matter problems. The most common fractions of particulate matter measured include PM_{2.5}, PM₁₀, and total suspended particles (TSP). The focus of this study was to evaluate relationships between PM_{2.5}, PM₁₀, and TSP concentrations specific to the Hanford Site, near Richland, Washington. Measurements of PM_{2.5} and PM₁₀ concentrations continued while additional measurements of TSP were made over several summer months. Four sampling locations on the Hanford Site were used to compare spatial differences in the data. Comparison of the data revealed a strong linear correlation between PM₁₀ and TSP for the time period evaluated. The correlation between PM_{2.5} and TSP was not as strong, and indicated that local sources rarely were above background measurements. This was supported by the correlation of ground level PM_{2.5} with PM_{2.5} concentrations measured on a near by mountain.

Economic Variability in the Hanford-White Bluffs Irrigated Farming District at the United States' Department of Energy's Hanford Site: A Historical Archaeological Analysis of 20th Century Farms in Southeastern Washington. STEPHANIE SIMMONS (*Central Washington University, Ellensburg, WA 98926*) ELLEN PRENDERGAST-KENNEDY (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Written history alone has proven not to be a reliable source to understanding the past. But when archaeological data is combined with historical records a much clearer picture emerges. This study used

an historical archaeological approach to compare the archaeological record with United States Government historic record to explore the amount of economic variation in early 20th century Hanford-White Bluffs area farmsteads, which are now located in the United States Department of Energy's Hanford Site. Thirty-six farms with archaeological remains were identified and compared to the historically known price paid per acre for each farm. The results indicated there was no correlation between the archaeological and historical data sets. In addition, the data revealed little economic variation in the farms. The results either suggest that little economic variation is a reality, or that the sample size was too small. In addition to using a larger sample size, future studies should improve the quality of the archaeological data through excavation and improve the historical data through a better understanding of appraisal methods.

EPA WA 2-18 Endocrine Disruptor Screening Program: an ERULF Students View. ARTHUR PRINCIPE (*Rochester Institute of Technology, Rochester, NY 14623*) MICHAEL L BLANTON (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Work assignment 2-18 is a contract with the U.S. Environmental Protection Agency (EPA) Endocrine Disruptor Screening Program to develop a protocol for screening chemicals in the environment that have the potential to have endocrine disruptive effects. In this study, we evaluated three test protocols using four different pre-selected chemicals to determine which protocol might be the most appropriate. We used the fathead minnow (*Pimephales promelas*) as a test organism under the following test scenarios: EPA 21-day reproductive test, EPA 14-day reproductive test, and OECD 14-day non-reproductive test. Test set-up involved following the protocols for each test as to the number of concentrations, replicates, number of fish per tank, tank set-up, and pre-validation activities, if required. A closed-system pipe apparatus was created to ensure contaminated water was kept separate from the bath water. Daily water quality observations included taking measurements of ammonia, pH, temperature, and dissolved oxygen. Daily test activities included observations of fish behavior, fecundity counts, and animal husbandry tasks (feeding, tank cleaning, euthanizing, as needed). We also collected and hatched eggs to assess survivability. Evaluations were made as to the necessity of tasks, labor requirements, and means of making the protocols more efficient and cost-effective. Significant to this program was the termination of organisms and collection of blood and gonads. Blood was tested for five chemicals; gonads were weighed to determine gonadosomatic index (GSI) levels. Data were entered into an Access database using a web-based system.

Frequency of Occurrence and Optical Depth Properties of Jet Contrails Over the Pacific Northwest. NICOLE GRAGEDA (*Walla Walla Community College, Walla Walla, WA 99362*) THOMAS ACKERMAN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The effects of jet contrails on earth climate have not been extensively studied, especially in the northwestern United States. The extent of their impact varies with their frequency of occurrence and optical depth properties. Currently it is not understood if contrails have an overall warming or cooling effect on the earth. Analyses of contrails above southeastern Washington State were made using the Total Sky Imager (TSI) to keep a visual record of contrail activity and also the Normal Incidence Multifilter Radiometer (NIMFR) to track the direct normal solar irradiance. The frequency of contrail occurrences was also monitored. The optical depth of selected contrails was calculated by first subtracting the ozone and Rayleigh (molecular) optical depths of the atmosphere, compensating for aerosols, and then adjusting for forward scattering. Jet contrails occurred infrequently around PNNL during the time period studied and were often associated with other clouds making a detailed analysis difficult. Contrails occurred on 29 days during the study, with 5 being suitable for a detailed analysis. The contrails typically had an optical depth of .3 or less. More research into jet contrails is needed before any definite inferences can be made. An extended analysis using LIDAR (Light Detection And Ranging) and monitoring humidity is warranted.

Hanford Roadside Breeding Bird Survey Analysis: 1988-2003.

SHELLEY DEBOER (*Northwest Nazarene University, Nampa, ID 83686*) MARY ANN SIMMONS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The Hanford site occupies a remnant shrub-steppe habitat in eastern Washington state. Over the past 16 years bird populations have been monitored by taking roadside surveys along four routes representing distinct communities on the site. The purposes of this study were to determine which species have been using the site and to analyze the collected data to determine the trends in the abundance of shrub-steppe, breeding birds. Sixteen species were selected for trend analysis; the four most abundant were Western Meadowlarks (*Sturnella neglecta*), Horned Larks (*Eremophila alpestris*), Black-Billed Magpies (*Pica hudsonia*), and Common Ravens (*Corvus corax*).

A log-linear regression model was used to evaluate the trend in annual data. The data used for trend analysis was found by computing the mean count of each species found in April, May, and June of each year. The analyses revealed that several species have declined significantly in abundance on one or more routes. Of the species that were used in the analysis, none showed an increasing trend in abundance. Western Meadowlarks have declined significantly on all four routes, while Horned Larks and Black-billed Magpies have declined significantly on only one route. These results will be instrumental in monitoring and assessing the ecological health of the Hanford site.

Historical Trends in Ground Water Contamination at the Hanford Site: T, TX, and TY Tank Farms. MICHELE SMITH (*Southern Nazarene University, Bethany, OK 73008*) DUANE HORTON (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Since the late 1940's, groundwater samples have been taken from wells near tanks, cribs, and trenches on the Hanford Site, which contain waste from the production of plutonium during the Manhattan Project. Certain contaminants have entered the groundwater as a result. It is necessary to know if the distribution of contaminants can be traced through history, thus helping determine the sources of contamination and potential future distribution. The T, TX, and TY tank farms were chosen for this research. A group of wells, located in and around this area, were selected along with two constituents, nitrate and tritium. Nitrate and tritium concentrations in groundwater were extracted from a database and organized by constituent and year of measurement. These data were then used to make plume maps. From these maps it was determined that the contaminants were not detectable past the northeast corner of the 200 West Area because of a paleo flood channel. This more permeable channel causes the water to move faster and increases dilution. Sources of contamination were seen to fluctuate with use of certain facilities. Locally, specific cribs and tile fields can be identified as contaminant sources, but no evidence for a tank source was found. After the maps were made, ratios of contaminant concentrations were used in order to determine where contaminants originated. No conclusions could be made from the ratios. This could be the result of several factors: regional plumes of contaminants; distribution of similar wastes to tanks, trenches, and cribs; and questionable data values. This project provided new information about contamination at the T, TX, and TY tank farms. Some contaminant sources were identified directly and it was found that the geology of the Hanford Site is affecting contaminant distribution.

Improving Modeling of Iodine-129 Groundwater Contamination Plumes Using the System Assessment Capability. JACQUE DIRKS (*Northland College, Ashland, WI 54806*) WILLIAM E. NICHOLS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Years of production of radioactive materials at the Hanford Site in southeastern Washington State has resulted in contamination of surface, subsurface, and surface water environments. Cleanup of the site has been aided by various tools, including computer software used to predict contaminant migration in the future and estimate subsequent impacts. The System Assessment Capability (SAC) is a total systems tool designed to simulate the movement of contaminants from all waste sites at Hanford through the vadose zone, the unconfined aquifer, and the Columbia River. Except for iodine-129, most of the contaminants modeled by SAC have acceptably matched field measurements. The two most likely reasons for the inconsistency between the measured field data and SAC modeled predictions are an underestimated inventory and an overestimated sorption value (Kd). Field data tend to be point measurements taken from near the surface of the unconfined aquifer. Thus, the depth of the iodine-129 contamination plume on the site is not well characterized. Geostatistical analyses of the measured data were conducted to determine the mass of iodine-129 for four assumed plume depths within the unconfined aquifer. Several simulations for two different Kd's using the initial SAC inventory were run to determine the effect of an overestimated sorption value on SAC modeled predictions. The initial SAC inventory was then increased for the two different Kd's to determine the influence of an underestimated inventory on SAC modeled predictions. It was found that evidence for both an underestimated inventory and for an overestimated sorption value for iodine-129 exist. These results suggest that the Kd for iodine-129 should be reevaluated and that a more complete inventory must be generated in order to more accurately model iodine-129 groundwater contamination plumes that match available field data.

Phosphate Precipitation for Remediation of Lead-Contaminated Groundwater. LAURA BEGAY (*South Mountain Community College, Phoenix, AZ 85042*) JONATHAN P. ICENHOWER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Absorbance spectroscopy was used to monitor the precipitation of lead-phosphate minerals from groundwater under a range of lead and phosphate concentrations, and with polyphosphates of varying chain length. Absorbance measurements were conducted to determine the extent and time dependency of lead-phosphate precipitation in groundwater. Sodium tribasic dodecahydrate (monophosphate) $[\text{Na}_3\text{PO}_4 \cdot 12\text{H}_2\text{O}]$ was shown to react instantaneously and the maximum absorbance was obtained in less than 20 minutes. The hydrolysis kinetics of sodium triphosphate (tripolyphosphate) $[\text{Na}_5\text{P}_3\text{O}_{10}]$ hindered precipitation and the absorbance continued to increase through two hours of monitoring. Powder X-ray diffraction (XRD) was performed to identify the resulting precipitates as $\text{Pb}_9(\text{PO}_4)_6$.

The Columbia Basin Hydroelectric System: Its Influence on Anadromous Fish and Technologies to Aid in their Recovery. ABIGAIL CAPETILLO-ISENBERG (Western Washington University, Bellingham, WA 98225) DAVID GEIST (Pacific Northwest National Laboratory, Richland, WA 99352).

The Columbia River Basin is the most hydroelectrically developed river system in the world with more than 400 dams. Obstruction of fish movements by dams continues to be the major environmental issue facing the hydropower industry in the United States. While hydroelectric dams provide water for irrigation, electricity and flood control, they also block upstream fish migrations, cutting some stocks of fish off from their historical spawning grounds and severely curtail reproduction. Also, downstream migrating fish may be entrained into the turbine intake flow and suffer injury or mortality. Salmonid habitats in the main-stem Columbia and Snake Rivers have changed dramatically during the past 60 years. Advances in the electronics industry have enabled scientists to develop sophisticated telemetry methods to monitor the locations, behavior, and physiology of free-ranging aquatic animals. Radio and acoustic telemetry provides researchers the ability to detect and record fish movement without interrupting their seasonal, cyclic movements in the river system. These technologies are aiding researchers in the recovery of Columbia River salmonids.

The Future Effects of Methane and Nitrous Oxide Emissions from Chinese and Indian Agriculture. REYLYNNE WILLIAMS (South Mountain Community College, Phoenix, AZ 85042) MICHAEL J. SCOTT (Pacific Northwest National Laboratory, Richland, WA 99352).

Methane (CH_4) and Nitrous Oxide (N_2O) are important greenhouse gases, which contribute to global warming and climate change (Cole et al, 1997). Methane emissions are produced from waste management, net emissions from agriculture, rice cultivation, biomass burning, industry and fossil fuel combustion, and other various sources (Brenkert, 2000). Nitrous oxide emissions evolve principally from fertilizer use, agricultural waste burning, decomposing animal waste, and land use changes (Brenkert, 2000). Agriculture dominates as the main source of methane and nitrous oxide emissions (Cole et al, 1997). Research efforts have modified the emissions framework of the Intergovernmental Panel on Climate Change (IPCC) Phase II guidelines (IPCC 1997), developed by the IPCC and the Organization for Economic Cooperation and Development (OECD) for national emissions inventories, and linked it to operate with Pacific Northwest National Laboratory's Agriculture and Land Use (AgLU) Model. We searched various literatures, and web-based information from national and international statistical sources was used with the Agriculture and Land Use (AgLU) model. Data were obtained from simulated technology and market relationships governing methane and nitrous oxide emissions from Chinese and Indian agriculture for the purpose of conducting policy-sensitive emissions modeling of these greenhouse gases. This paper shows that, the context of moderate climate change, improvements in fertilizer application efficiency and animal management make it possible to reduce the total agricultural nitrous oxide emissions anticipated in 2080 can be held in India to the levels recorded in 1995, (an 8 % reduction), but this is not likely in China, where nitrous oxide emissions would rise by about 35 percent.

GENERAL SCIENCES

Becoming a Science Writer. RHIANNA WISNIEWSKI (University of Illinois, Urbana-Champaign, IL 61801) DAVE BAURAC (Argonne National Laboratory, Argonne, IL 60439).

Writing about scientific and technical developments and their applications promises to be an interesting and fulfilling career. Learning how to translate technical and scientific jargon into simple understandable concepts for the everyday person is a valuable skill that my time as a science-writing intern here at Argonne has helped to develop. The technical nature of the articles I wrote as well as the coaching and accessibility of my mentor and other editors helped me to improve my researching and editing skills and to become a much better writer. Pho-

tophography, Web design, HTML, and public relations skills are just a few of the things that I did not expect to learn during my internship at Argonne National Laboratory. I was challenged by both my individual assignments and my work throughout the internship as a whole. I always had multiple assignments to balance at any point during my employment, and this helped to teach me how to meet deadlines and how important it is to use time efficiently. I have already completed my undergraduate education, but this internship has helped persuade me to continue my education, perhaps getting further degrees in journalism or public relations.

Calculation of the Positron Emitter Production During Proton Radiotherapy and Their Cross Section Data Dependence. LINDSAY SMITH (Louisiana State University, Baton Rouge, LA 70820) JOANNE BEEBE-WANG (Brookhaven National Laboratory, Upton, NY 11973).

The previous work at BNL has demonstrated that PET is a potentially powerful tool for quality assurance of proton radiation therapy (RT), which is especially important when treating inhomogeneous organs where the calculation of the expected dose distribution for treatment planning is more difficult. In this paper, an analytical calculation is presented showing the yield of positron emitters produced by proton beams up to 250 MeV in conjunction with the Monte Carlo simulation predictions in the previous work. The predictions of the positron emitter distributions are produced through analytical formulas and simple calculations, which can be used as a benchmark for detailed experiments or simulations. It is also demonstrated that the calculation results of the positron emitter production distribution is strongly depend on the nuclear reaction cross section data for given proton beam flux and target elemental compositions. The emphasis of this work is to determine quantitatively the differences in the calculated distributions resulted from four different sources of the nuclear reaction cross section data.

Using X-ray Crystallography to Determine the Structure of Lysozymes. EDWARD BELL (South Carolina State University, Orangeburg, SC 29117) BRIAN MURFIN (Brookhaven National Laboratory, Upton, NY 11973).

Lysozyme, an enzyme found in human tears, mother's milk, mucus, saliva and secretions is studied to determine its potential to cure AIDS. Scientists noticed that the enzyme stops the spread of HIV. They suspect lysozyme prevents HIV from raiding the immune system by collapsing the outer membrane of the virus. Alexander Fleming discovered lysozyme, to understand whether natural substance found in the body can combat destructive bacteria, and viruses. After numerous trials against perilous bacteria, lysozyme was concluded to be active against inert bacteria. Later, research has shown that when the activity of lysozyme is adjusted, it is active against destructive bacteria such as *E. coli*, by compromising its properties against the bacteria's outer membrane. Lysozyme has been examined extensively through X-ray crystallography and diffraction to understand the structure of lysozyme; relate how active the protein is when adjusted according to size, level of pH, temperature, etc.; and how can it be applied in the medical field. Through research, mathematical equations have been developed to express the lysozyme's behavior. Additional studies on lysozyme joining forces with other proteins or enzymes are observed to suggest its ability to fight HIV or AIDS. With more research of lysozyme, it might help scientists to develop remedies against AIDS, and other viruses or bacteria.

Cosmic Ray Detection. ANGELINA BUSTOS (California State University, Fresno, Fresno, Ca 93612) PEGGY MCMAHAN (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The objectives of the Cosmic Ray Detection Workshop were to understand the source and nature of cosmic rays, be able to use a cosmic ray detector for experiments, learn how to build a cosmic ray detector, learn why cosmic rays are important to space and earth, and be able to explore ways to use a cosmic ray detector in the classroom to teach standards based content. We began by understanding the background and nature of what cosmic rays really are. We learned that even though they are being detected here on earth by specialized detectors, their origins remain to be a mystery to all who study them. The experiments that have been done have only been able to determine the direction these rays are traveling when they hit the earth. Primary cosmic rays come in from interstellar space, hit our atmosphere and collide with other particles that cause a cascade of secondary particles that then get detected at the earth's surface. Through use of hands-on and internet based activities we were able to understand how charged particles can be detected and why a stacked scintillator that counted coincidence events was the best way to approach the problem of counting cosmic rays. We participated in construction of the detector as a group. We were then able to test our Berkeley Detector, troubleshoot a shorted circuit, and begin to take readings. We then were able, using a GPS system, to measure cosmic ray counts versus altitude. We took mea-

surements at the Berkeley Marina (sea level), at LBNL (824 ft.), half way up Mt. Diablo (1505 ft.), at the summit of Mt. Diablo (3859 ft.). With this data we concluded and reaffirmed prior studies that the higher you go in elevation, the more cosmic rays you will encounter. These particles that shower down upon us are important to study because of the effects they may have on astronauts and equipment in outer space, air craft employees, and the effects that solar cosmic rays may have with changing solar weather.

Fat Finders: Inquiry-based Nutrition Activities for Grades 3-5. LYNNE CLOUGH (*Lesley University, Cambridge, MA 02138*) MARY CONNOLLY (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The mission of the Family Health project is to improve student, teacher, and family understanding of health issues and the science behind them. Having developed and tested activities for students to explore sugar, in Sugar Sleuths, a need arrived for similar activities about fat. I began to research fat in the diet, finding that there is much new information and subsequent confusion in the popular press. I had to decide what the students need to know, how they were going to learn it, and how I could compile a set of activities that would reflect the learning cycle, incorporating science inquiry. I wrote a set of inquiry-based activities called Fat Finders for grades 3-5. These activities follow the learning cycle where students are first engaged, and invited to then explore, explain, and extend their understandings.

FTIR Applications: Fingerprinting. BRANDY MURRAY (*Fresno City College, Fresno, CA 93741*) ROLLIE OTTO (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

The objectives were to learn the electromagnetic spectrum, why infrared is used to study molecules, use an FTIR spectrometer, and collect infrared data on fingerprints. The electromagnetic spectrum is the entire range of wavelengths or frequencies of electromagnetic radiation extending from gamma rays to the longest radio waves and including visible light. Infrared spectroscopy is used to study chemical composition. Through this method, one can detect interference patterns of infrared waves of very small samples (less than 10 μm when using a synchrotron). We used Fourier-transfer infrared spectromicroscopy to collect data on fingerprints, and then analyzed the fingerprints to find remnants of items the subject had recently touched (such as hair gel or lotion). We were also able to analyze a sample of UV latent fingerprint powder, left on a vehicle that a suspect had attempted to steal after a forensics team had dusted for fingerprints, to test for its chemical composition. We used both the thermal global and synchrotron sources and found that the synchrotron was able to pin-point very small areas of just several microns, whereas the global source only allowed us to get a general idea of the spectra for a size of about 100 microns. Ultimately, using the synchrotron, we were able to determine that there was indeed a pink pigment, and hematite in the sample, and that the sample absorbs water. These findings are reasonable, since the sample has to absorb water in order to attach to a print so forensics teams can see the print (anywhere there is no moisture, the dust would not adhere). Also, the remnants on the vehicle had a pink-tone, so it makes sense that both the pink pigment and hematite (which is red to brown in earthy forms, and minerals are often times used in powders) were found.

Infrared Spectroscopy. RAUL OSUNA (*California State University Fresno, Fresno, Ca 93740*) ROLLIE OTTO (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Infrared Spectroscopy helps us find compound in many things such as materials, gases, and living cells. Our experiment was to learn the importance of infrared radiation to the modern study of molecules. Infrared radiation comes from many sources, most of which come from the sun and we feel as heat. Using the Infrared Beam line at the Lawrence Berkeley Lab's Advance Light Source we were able to find compounds in materials. Our apparatus was a Fourier Transform Infrared (FTIR) Spectrometer. We learned how to use the FTIR spectrometer and understand its associated spectra. Aside from the sun being a great provider for infrared we used two sources that are man made. The Tungsten source provides with a good spatial resolution and it is used in large samples. Also it is possible to use a synchrotron for better spatial resolution or smaller samples. Through a series of other workshops we learned about the electromagnetic spectrum and its associated wavelengths. The FTIR spectrometer allowed us to study different wavelengths of the infrared hence infrared has a lot of wavelength. From this we were able to collect data on the percentage of infrared light that made it through the sample. Different samples absorb different percentages of infrared. By comparing our spectra to a database we were able to find the compounds in our sample.

Analysis of the Native American Anemometer Loan Program. AL-EXANDER ISRAEL (*Northern Arizona University, Flagstaff, AZ 86011*) LISA DECKER (*National Renewable Energy Laboratory, Golden, CO 89401*).

Wind power was the fastest growing renewable energy in the 1990s. The majority of this growth has been in Europe, due to the high cost of conventional energy. Much of the wind resource in the United States has not been tapped. 96 million acres of U.S. land belong to 700 Native American and Alaskan tribes. The Native American Anemometer Loan Program provides Native American and Alaskan Indian tribes with the proper equipment to do a wind assessment test. Wind Powering America (WPA) through the National Renewable Energy Laboratory (NREL) administers the Native American Anemometer Loan Program. The program gives the tribe 14 months for the wind assessment test, 1 month for shipping and installation, 12 months of monitoring, and 1 month to disassemble and return the equipment. The equipment consists of NRG Systems 20 meter wind explorer kit. The kit includes a 20-meter tower, installation kit, anemometer, wind vane, data logger, datalog, and data-plug reader. The data from the site are logged onto an NRG Systems DataPlug; each site receives two NRG Systems DataPlugs. Each month the DataPlug is sent to WPA for processing. An NRG Systems DataPlug reader is used to read the data of the DataPlug. And NRG Systems Wind Data Retriever program is used to convert the data into readable data on a computer. Microsoft Excel spreadsheets are used to create a monthly summary of the wind resources. The spreadsheet is then analyzed for problems and a copy is sent to the tribe. After 12 months of monitoring, a final report is created. The final report analyzes the data for the entire 12 months, and determines if the tribe's intentions are feasible. As a result of wind assessment testing, some sites have gone on to install wind turbines on their land. The Rosebud Sioux have installed a 750 kW wind turbine on their reservation to provide electricity for a casino and motel. The wind assessment test done on their land helped the tribe receive the United States Department of Energy's cooperative grant. Many Native American and Alaskan tribes in the United States have abundant wind resources in their area, but have not taken advantage of them. Wind Powering America's Native American Anemometer Loan Program is an excellent method to test for wind resources.

Biodegradation of Aromatic Compounds by Soil Microorganisms. LINDSEY BUEHLER (*University of Northern Colorado, Greeley, CO 80631*) STEVE PHILLIPS (*National Renewable Energy Laboratory, Golden, CO 89401*).

Byproducts of the thermo-chemical biomass conversion process include several aromatic compounds that are released in an aqueous effluent. Removing these aromatics from the water would eliminate hazardous waste storage or costly disposal. One way to remediate the aromatics from the water is to introduce indigenous microorganisms with the capability of degrading the compounds. To find a microorganism or microbial consortia capable of degradation, two soil samples were collected from a local site that may be contaminated with cresol, one of the aromatic constituents found in the aqueous effluent. Soil microorganisms that may have metabolic pathways for degrading cresols or phenol were selected for and the concentrations of the compounds were measured using gas chromatograph-mass spectroscopy (GCMS). To identify the possible candidates for bioremediation, polymerase chain reaction (PCR) was performed using universal primers for the 16S rRNA gene. A 16S rRNA clone library was constructed and restriction digestion, along with other tools, was used to differentiate between clones. The results of this study are inconclusive because the internal standard used was not consistent; therefore, we are unable to conclude whether any of the identified microorganisms in the soil samples are capable of metabolizing the aromatics as a carbon source and degrading the compounds from the waste water. We recommend additional experimentation on the internal standard (4-bromofluorobenzene), refinement of the extraction protocol, and replication of the experiment in larger quantities. We also suggest further investigation into the requirements and capabilities of the identified microorganisms so that an in-situ (on site) bioremediation step can be developed and directly incorporated in the biomass conversion process.

Method Validation; Soxhlet Extraction of Corn Stover. JENNIFER PRATT (*Lehigh University, Bethlehem, PA 18015*) BONNIE HAMES (*National Renewable Energy Laboratory, Golden, CO 89401*).

In the cascade of analytical procedures, biomass analysis of corn stover requires that nonstructural materials first be removed to prevent interference with downstream lignin, structural sugars, and protein analysis procedures. Soxhlet water extractions remove such interfering materials as non-structural sugars and soil. Current NREL Laboratory Analytical Procedures (NREL LAP10) call for a 24-hour water extraction period (100-120 cycles). This procedure could be improved with information

on what water-soluble materials are being removed and when, so that compound-specific extraction times could be listed. Method validation identified steps to extract all glucose, sucrose, and other compounds of interest from biomass. Sugar content of the biomass extracts was monitored with a YSI Bio-Analyzer and Enzymatic Test Kits to determine the effectiveness of the extraction over a 48-hour period. Ash and nitrogen-containing compounds were also measured. Results demonstrated that the extraction processes called for in LAP10 could be refined into a more time-efficient process.

A Pilot Program to Assess Safety and Health Issues in Office Settings. MEREDITH HOLDER (*Lincoln Memorial University, Harrogate, TN 37752*) JOHN C. CZACHOWSKI (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Developing a system to identify safety and health hazards that the office environment poses for the employees of the Engineering Science and Technology Division of Oak Ridge National Laboratory (ORNL) was the aim of a pilot study this summer. Reviews of safety records indicated that ergonomic injuries, related to office exposure, were the primary source of lost time injury in the Division. Therefore, a program aimed at inspecting the workplace of each administrative staff member in the Engineering Science and Technology Division (ESTD) for potential problems was implemented. The initial step was to develop and utilize an Office Area Safety Inspection Checklist based on the ORNL Standards Based Management System and Occupation Safety and Health Agency (OSHA) guidelines. This tool aided in recognizing the hazards that one might expect to find in an office and was crucial for assessing these work areas. The checklist assisted the observer in evaluating different aspects of the office area and provided a form of documentation of each evaluation. The information attained from each observation was input into a Microsoft Access database. Visual reports created from the database charted the percentage of totals of hazards found in each category. After observing a significant portion of the employees of the Engineering Science and Technology Division, particular trends of safety issues began to emerge. As of July 17, 2003, 228 self-assessments were completed, and sixty-four total hazards were found. Among these hazards, twenty-two, or 34%, were ergonomic related hazards. This was a significant percentage compared to the percentages found in other hazard categories. It indicated that poor ergonomic factors and repetitive tasks were a contributing factor to work-related injuries. As more assessments are completed in the future, a clearer representation of the safety and health hazards in the division should transpire. Therefore, more investigation, time, and money are warranted in order to improve the safety and health of ESTD's office environments.

Gas Detection Module Using Microcantilever Sensors. FELESHIA BALLOU (*Virginia State University, Petersburg, VA 23806*) JAMES HARDY (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The project objective was to develop a stand-alone, portable, telemetric, low power and low cost microsensor platform for detecting gases like Carbon Dioxide, CH₄, H₂ and NO_x, using MEMS fabricated array of microcantilever devices. These microsensors were coated with a gas sensitive chemical that changes the cantilever electrical capacitance with small, ppm level variations in the amount of ambient gas present. The resulting small femtoFarad capacitance changes were sensed and amplified using a specially developed GS2 microelectronic integrated circuit. Special chemicals and polymers, like 3-aminopropyltrimethoxysilane, specifically sensitive to Carbon Dioxide gas, were prepared using sol-gel chemistry and then carefully applied in picoliter quantities selectively on top of the 50 x 100 microns microcantilever beam using piezoelectric driven Microjet nanofluidics technology. The GS2 ASIC chip was fully tested and characterized. The integrated test results proved that the GS2 chip was fully functional for its filter, offset and gain specifications and that the coated microcantilevers were capable of detecting ppm level changes in CO₂ concentration. Humidity and Temperature microsensors and Infrared IR radiation detectors are also being incorporated into the MEMS microchip. A telemetry transceiver module allowing wireless RF transmission of the data using adaptive spread-spectrum protocol is also being developed. The microsensors and the transceiver module will be interfaced to the GS2 ASIC; the total microelectronics package will be integrated into a pocket size gas detection unit that operates on batteries, consuming only milliWatts of power. The output of the detected Carbon Dioxide, Relative Humidity and Temperature levels are to be incorporated into the DOE Zero Energy Building (ZEB) HVAC Energy Management computer controlled system to reduce energy cost and increase efficiency. Other applications would include greenhouse gases monitoring for environmental protection, airplane and automobile air conditioning control, internal combustion engine energy efficiency improvement and industrial gas analysis. Another important application would be in Homeland Security where human presence in a room could

be detected and the information transmitted wirelessly over the sensor network. By incorporating microcantilever Hydrogen gas detectors, the microsensors can also be used in fuel cells and in hydrogen transport and storage systems.

Safety Evaluations of Engineering Science & Technology Division Laboratories at Oak Ridge National Laboratory. CHARLES COOMER (*University of Tennessee, Knoxville, TN 37919*) JOHN CZACHOWSKI (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*). Conducting world-class research involving a wide range of physical and chemical hazards while maintaining an environment of safety for the researchers and support staff is the driving factor of all the work at the Oak Ridge National Laboratory. In Engineering Science and Technology Division the task of maintaining this declaration was supported this summer by a pilot program consisting of two parts. The two parts: observation of laboratories and tracking known hazards. The observation portion was preceded by a review of the Research Safety Summary (RSS) to become familiar with the hazards in the labs that are currently present. In the RSS each hazard is identified and proper controls set in place. It was necessary for the observer to observe the researchers and their assistants while they were performing the research work to make sure that they are following the proper procedures for their jobs as outlined in the RSS. A concentrated effort was made to observe the workers in their laboratories from an Environmental, Safety, and Health outlook and to include an engineering perspective. This included participation in new facility safety walk through and experimental design reviews. It was also necessary to keep a running record of the hazards and known violations. This was achieved by developing a database using Microsoft Access. The purpose of the database was to keep track of the laboratory and office safety assessments. First, the computer programming language, SQL, needed to be developed. The database was setup for data entry, search criteria, statistics, and report printing with charts and graphs. The reports were for monthly, quarterly, and yearly statistics. As of July 16, 2003, based on 220 offices assessed, the results found are 55 hazard concerns in the researcher and administration offices for the Engineering Science and Technology Division. Of these 55 concerns found, the largest majority have been ergonomic problems at 33%. The numbers for the laboratories has not been calculated at this time. This Pilot project will be complete by mid August. The safety of the researchers and administration has been good overall, but an improvement in ergonomic hazard recognition and remediation is identified as an opportunity for improvement.

Erratic Behavior on Rattlesnake Mountain, Hanford Reach National Monument, South-Central Washington. ELYSIA JENNETT (*Northern Arizona University, Flagstaff, AZ 86011*) BRUCE BJORNSTAD (*Pacific Northwest National Laboratory, Richland, WA 99352*).

A study of the ice-rafted debris has been performed in a long-protected, sparsely vegetated, 17 mi² area on the NE flank of Rattlesnake Mountain, now part of the Hanford Reach National Monument. The objective of this study was to catalog ice-rafted debris on Rattlesnake Mountain and look for trends in their distribution. Ice-rafted debris is of three types: 1) isolated erratics, 2) erratic clusters, and 3) bergmounds. Locations of erratics with >1 ft² area (planview) and bergmounds were recorded using a hand-held GPS. Additional information was gathered on: 1) elevation, 2) lithology, 3) size, 4) roundness, 5) shape, and 6) surface characteristics of erratics. Greater than 95% consist of rock types other than indigenous basalt; >75% being of granitic composition. Approximately 30% of erratics, perhaps derived from older pre-Wisconsin floods, are strongly weathered. The distribution of erratics is non-uniform and their overall size and frequency decreases with elevation. Decreases in the number of erratics with elevation can be explained by an increasing number of smaller floods. Decreases in size may be due to either: 1) larger floods producing smaller icebergs, or 2) large icebergs, capable of rafting more and larger debris, becoming grounded well away from the ancient lakeshores. Since bergmounds are generally absent above 1000 ft, we prefer the later explanation. Erratics appear to concentrate along the N sides of a series of NE-trending gullies within the study area. Variable flow velocities across this uneven surface may have created eddies, forcing icebergs to collect in the deeper and quieter waters along the backsides of these gullies.

Into Scientific Exploration. RILEY O'BRIEN (*Princeton Theological Seminary, Princeton, NJ 08540*) ROBERT KAITA (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

This paper proposes an innovative approach to implementing the inquiry based teaching model into the science classroom. In this approach, a student's natural tendency to ask deep, philosophical questions is encouraged, especially among younger students. Children are like scientists in that they are naturally curious and seek to explore answers to larger global questions. These questions are often discouraged, since

the questions are often deemed unscientific, and simple answers are nonexistent within the boundaries of science. In the proposed approach, a student's global questions are viewed as motivation towards authentic exploration. Under the teacher's arful guidance, students learn to reformulate their questions into narrowed down ones that are manageable within the realm of science. Because the students are genuinely involved intellectually in the process of exploring answers to their own questions, they acquire more than scientific facts and information. Students also learn the process and methods of science, the limitations of these methods, and critical thinking skills essential not only for future scientists, but for all responsible citizens. Also included is a module composed of a sample guided question as may be asked by an eighth grade student. The module starts with a typical deeply philosophical question, and ends in scientific questions and a science activity.

MATERIALS SCIENCES

Air Oxidation Kinetics of Zircaloy-4 Cladding. MICAH BAQUERA (University of Texas at El Paso, El Paso, TX 79968) W.K. SOPPET (Argonne National Laboratory, Argonne, IL 60439).

Air oxidation experiments were done on Zircaloy-4 with pretreatments to evaluate the kinetics of oxidation as a function of temperature, time, and pretreatment. Rings, capsules and tubes were fabricated from Zircaloy-4. Capsules and tubes were pretreated in a steam environment at 550°C for 140h to achieve an initial oxide thickness of ~30µm. These capsules were then placed in radiant furnaces at temperatures ranging from 300°C-900°C. The capsules were periodically removed, measured and weighed to calculate follow on oxide thickness. At the conclusion of the tests capsules were sectioned for metallography. Tubes of Zircaloy-4 with pressure fittings were used for oxidation tests with an internal pressure. Argon gas was used to pressurize the tubes in a radiant furnace at temperatures of 600°C, 700°C, and 800°C. Tests were run until the tubes experienced failure due to rupture. Volume changes were measured, and at the conclusion of the tests tubes were sectioned for metallography. Ring samples were exposed to a H₂ atmosphere at 320°C for periods of 6h -92h. The rings were weighed at the end of each run to measure the amount of hydrogen uptake. From the air oxidation data, oxidation rates and correlations of oxide thickness as a function of temperature will be created. This can be used for analyzing its behavior in a variety of oxidizing conditions. Rates at which tubes fail will be developed and analyzed to see which of the competing processes, oxidation vs. expansion due to pressure, is dominant at different temperatures. Hydrogen uptake has been variable within the same material. However, more data will be acquired, for use in evaluation of hydriding on subsequent oxidation.

Catalysts for Autothermal Reforming of Hydrocarbon Fuels. ALEX MARTINSON (Luther College, Decoah, IA 52101) JENNIFER MAWDSLEY (Argonne National Laboratory, Argonne, IL 60439).

Before the United States realizes a hydrogen economy, many challenges must be overcome. Not the least of these challenges is the production of hydrogen. This project explores the feasibility of reforming gasoline into hydrogen through a process called autothermal reforming. Autothermal reforming reacts oxygen, steam, and hydrocarbon fuel to produce hydrogen and carbon dioxide. Efficient autothermal reforming requires the use of a catalyst as well as the optimization of several reaction parameters. Catalysts were prepared that consisted of transition metals deposited on yttrium-stabilized zirconia (YSZ) supports by incipient wetness impregnation. Catalysts were tested under autothermal reforming conditions at various temperatures for a given fuel mixture. It can be concluded from these studies that the performance of Rh-based catalysts is superior to catalysts containing Pd or Ir. Doping YSZ with 10% alumina (Al₂O₃) may increase the performance of transition metal catalysts in the short-term but results in decreased performance in longer-term tests. This decrease in performance is in spite of the smaller loss in surface area of the alumina-doped YSZ compared to the undoped YSZ.

Determine the Forward Glass Dissolution Rate of An Experimental Waste Glass Surrogate. ARTHUR KUEHL (University of Arizona, Tucson, AZ 85719) STEVE FRANK (Argonne National Laboratory, Argonne, IL 60439).

The forward dissolution rate of a surrogate glass material (low-activity reference material, LRM) provided by Argonne National Laboratory for an inter-laboratory study has been investigated at 70°C. The forward dissolution rate of the glass is being investigated by a single-pass flow-through (SPFT) test with the glass in a specified buffer solution (DI water with 0.004M LiCl+ 0.003M LiOH). A constant initial surface area is used, but different flow rates are tested to affect many flow rate to surface area ratios in order to construct a trend in the dissolution rate of

silicon from the glass as it depends on the flow rate. The final leachate solution was analyzed using Inductively Coupled Plasma - Atomic Emission Spectrum (ICP-AES) to determine the concentration of silicon in the glass. The final data was then used to determine the forward dissolution rate for the LRM glass, which turned out to be 8x10⁻⁶ g/(m²s).

Diameter Reduction of Diesel Fuel Injector Orifices Through Electroless Nickel Plating. JAMIE GRIFFITH (Whitman College, Walla Walla, WA 99223) JOHN WOODFORD (Argonne National Laboratory, Argonne, IL 60439).

Increasingly stringent diesel emissions regulations have caused a flurry of research into how to lower diesel engine emissions. It has been shown in a number of studies that decreasing diesel fuel injector orifice diameters can effectively reduce particulate matter emissions. Current production methods reliably produce 125 micron diameter orifices, but 50 micron diameter orifices are the industry goal. A number of techniques exist to create these smaller orifices, but are greatly hindered by their costs and production difficulties. In this study, we looked at coating pre-manufactured diesel fuel injectors with 200 micron diameter orifices with electroless nickel to reach the 50 micron goal cheaply and effectively. Three deposition techniques were tested, and after a number of trials, the 50 micron goal was reached and surpassed. The coating plated onto the steel of the injector smoothly and evenly and maintained the orifices original shape and structure. Extensive testing was carried out on the deposited coating including roughness and hardness measurements. The coating was found to be exceptionally adhesive and resistant to wear.

Growth of Carbon Nanotubes by Microwave Plasma Enhanced Chemical Vapor Deposition (PECVD). REYNALDO GARNICA (Florida State University, Tallahassee, FL 32304) GEOFFREY OTTENBERG (FSU, Tallahassee, FL 32310) JOHN CARLISLE (Argonne National Laboratory, Argonne, IL 60439) PETER J. GIELISSE (Argonne National Laboratory, Argonne, IL 60439).

Carbon nanotubes (C-NTs) of varying lengths and diameters were grown on nickel (Ni), iron (Fe), and a Ni-Fe alloy coated SiO₂ substrates. These metals were subjected to various synthesis environments that differed in temperature and gas flow rates towards the study of their effects on the C-NTs size, shape, quantity, and quality. The results indicate that Ni produced low quantities of C-NTs while Fe and the Ni-Fe alloy produced better results, with Fe outperforming the alloy. It was also found that higher quantities of C-NTs were produced at around 600°C. Preheating the film coatings at 800°C aided in film separation and in reducing the size of the particles on which the nanotubes nucleated. The outcome was a higher yield of nanotubes in shorter periods of time.

Low Cost Autothermal Diesel Reforming Catalyst Development.

JAMEEL SHIHADDEH (University of Illinois, Urbana-Champaign, IL 61820) DI-JIA LIU (Argonne National Laboratory, Argonne, IL 60439). Catalytic autothermal reforming (ATR) represents an important step of converting fossil fuel to hydrogen rich reformat for use in solid oxide fuel cell (SOFC) stacks. The state-of-the-art reforming catalyst at present is Rh based material which is effective but costly. The objective of our current research is to reduce the catalyst cost by finding an efficient ATR catalyst containing no rhodium. A group of perovskite based catalysts have been synthesized and evaluated under the reforming condition of a diesel surrogate fuel. Hydrogen yield, reforming efficiency, and conversion selectivity to carbon oxides of the catalyst ATR reaction are calculated and compared with the benchmark Rh based material. Several catalyst synthesis improvements were carried out including 1) selectively doping metals on the A-site and B-site of the perovskite structure, 2) changing the support from perovskite to alumina, 3) altering the method of metal addition, and 4) using transition metals instead of noble metals. It is found that the catalyst activity changed little with change in the A-site, while displaying considerable dependence on the B-site metal. Perovskite supports performed much better than alumina based supports. Ruthenium based catalysts have shown to achieve comparable efficiencies and hydrogen production to rhodium.

Novel Nanostructures Synthesized With and Without Templating.

AARON WITHERSPOON (Virginia Polytechnic Institute, Blacksburg, VA 24061) ZHILI XIAO (Argonne National Laboratory, Argonne, IL 60439). Nanostructures such as nanowires and nanotubes have attracted much interest due to their novel electrical, magnetic, and photonic properties. Quantum confinement, proximity interaction, and surface plasmon enhancement effects are a few of many extraordinary phenomena associated with nanowires and nanotubes. I report on two unique procedures that allow the fabrication of nanostructures through the electrodeposition of materials of interest on the surface of flat substrates and into nanopores contained in membranes. Electrodeposition, a common electrochemistry method to fabricate thin films and crystals,

reduces materials to a working electrode from a solution containing the associated ions by applying a voltage. By adjusting the applied voltage, the deposition process can be controlled. By adjusting the solution, the type of crystal structure that is grown can be controlled. We succeeded in fabricating nanostructures with novel shapes by electrodepositing materials of interest on flat surface of graphite. On the other hand, we utilized nanopores in anodic aluminum oxide (AAO) membranes to synthesize various nanostructures. The nanopores in AAO membranes is obtained through an anodization process, which converts aluminum foil with a thickness ranging from 0.25mm and 1mm into aluminum oxide through self-assembly, by placing the foil in an acid solution under a positive electric field. The self-organized pore diameters and pore-pore distances can be adjusted by changing the anodization voltage and acid concentration. These two approaches provide us unique ways to fabricate nanostructures with novel shapes. This paper will present detailed descriptions of these two techniques and sample nanostructures fabricated through them.

Proton Transfer in Super Ion Conductor, RbAg₄I₅. PINU STOUT (University of Texas at El Paso, El Paso, TX 79968) J.H. PARK (Argonne National Laboratory, Argonne, IL 60439).

There has been recent attention to further develop the hydrogen fuel cell. One boost to current fuel cell technology could be through the development of solid electrolytes for proton transfer. This study investigates the high ionic conducting solid, rubidium silver iodide (RbAg₄I₅), under a potential gradient from room temperature to 160°C. The conductivity of RbAg₄I₅ was measured and cyclic voltammetry performed in air, argon and hydrogen environments. From the conductivity measurements in 2% hydrogen environment, an activation energy, E_a = 0.063 eV was found. Compared to the E_a of BaCeYO, a high ionic conducting ceramic, the activation energy of RbAg₄I₅ is extremely low indicating energetic feasibility for proton (H⁺) migration in the solid. Thermodynamic considerations and cyclic voltammetry were employed in this study.

Molecular Dynamics Computer Simulation Study of Bulk and Surface States of Lead Silicate Glass. ERIC HEMESATH (Coe College, Cedar Rapids, IA 52402) L. RENE CORRALES (Pacific Northwest National Laboratory, Richland, WA 99352).

The evolution of ion diffusion relative to surface structure was characterized in lead silicate glass using molecular dynamics (MD) simulations. The classical potential model parameterized by Damodaran, Rao, and Rao (DRR) [Phys. Chem. Glasses 31, 212 (1990)] for lead silicate glass was used. Glasses were prepared using five distinct initial configurations and four glass forming algorithms. In previous MD work of bulk lead silicate glasses, the clustering behavior was not fully characterized. Here the persistence to clustering and details of molecular structure are determined, and their dependence on glass forming methodology is characterized. Also presented are changes in ion density distribution induced by surface exposure. The driving force to surface relaxation lies in the surface tension differences exhibited between pure SiO₂ and pure PbO. The cation with the lowest ionicity (I = z/a) moves to or stays at the surface, but no aggregation of species at the surface is found. Minimal changes are seen in the PbO cluster distribution in the presence of a surface.

Solid Oxide Fuel Cells: A Look into Cathode and Interconnect Research. AMY TRUJILLO (University of Missouri-Rolla, Rolla, MO 65401) TERRY CRUSE (Argonne National Laboratory, Argonne, IL 60439).

Solid Oxide Fuel Cells (SOFC) have the potential to become more efficient and environmentally friendly than present energy sources. SOFCs use hydrogen as a fuel, air as an oxidant and advanced oxygen-ion conducting ceramics to take advantage of a difference in partial pressure of oxygen separated by an oxygen ion conducting electrolyte and convert that energy to electricity, with only water as the byproduct. The average voltage output for one cell is one volt. However, fuel cells can be stacked in series using an interconnect to increase the working voltage and power output. The material and processing used for all components of the fuel cell are important to the end efficiency and power output. This paper discusses methods and procedures of testing different materials used for the cathode and interconnect.

Tip Fabrication for the Scanning Tunneling Microscope. ZOE PAUKSTYS (Illinois State University, Normal, IL 61761) DONGQI LI (Argonne National Laboratory, Argonne, IL 60439).

The STM allows imaging of a material surface structure through a tunneling current that is created between the conductive sample and a sharp, conductive tip. Having a sharp tip is essential for taking accurate STM images. The overall purpose of this project was to fabricate the tips that will be used for the STM; however it is with the specific goal to improve upon this process by consistently making sharp, well-shaped

tips. This was done by taking the existing set-up design and then reducing the time it takes for the circuit to cut off when the wire breaks, making it as short a time as possible and leaving the sharpest tips possible. To do this, a circuit was built that will served as a new power supply that allowed this shorter time to happen. The project originally began by the circuit being built and wired by hand, but after much difficulty a design was done by computer generating an outline of the circuit and then having it sent to have a board made with the wires applied directly onto the board. By doing this, the necessary components were attached to the circuit with minimal excess wiring.

Waveguide Properties of Amphiphilic Diblock Copolymers. ELAD HAREL (University of California San Diego, San Diego, CA 92130) HAU WANG (Argonne National Laboratory, Argonne, IL 60439).

The waveguide properties of various diblock copolymer systems are examined. Each diblock copolymer is composed of oligo(phenylene vinylene) covalently bonded to poly(propylene glycol) to form an amphiphilic rod-coil unit. These diblock copolymers are observed to undergo microphase separation with the addition of water to give rod and lamella morphologies. Optical Fluorescence Microscopy is used to characterize the waveguide properties of freestanding diblock fibers in a dilute THF/H₂O solution and 1 ± 0.2 mm wide diblock wires on a photolithographed template. Preliminary studies suggest optical transport properties in 20 ± 10 mm long fiber bundles.

Critical Current Analysis of a New Generation of Nb₃Sn Superconductors. LEONARD LUXAMA (The City College of New York, New York, NY 10031) LANCE COOLEY (Brookhaven National Laboratory, Upton, NY 11973).

In this work, the critical current distributions of a new generation of Nb₃Sn superconductors were derived from their voltage-current experimental data for analysis. The analysis of the critical current distribution provided details about the quality of the microstructure of the superconductors. The critical current distributions were found by taking the second differentials of the voltage-current data using a simplified least square method. A C programming language code was developed using this method to implement the calculations. The data files were plotted using 'Microsoft Excel'. Most of the data was not sufficient to complete the analysis, which has prompted changes in the experimental techniques. A complete distribution obtained for one sample was quite narrow, with the distribution width being ~5% of the average critical current. The average critical current was also about 35 A higher than the critical current obtained by a resistivity criterion. The implication of this analysis is that the state-of-the-art Nb₃Sn strands behave like uniform Nb-Ti accelerator magnet strands. However, this conclusion is not implied by the final microstructure of Nb₃Sn strands. A comparative metallographic approach will thus be the next phase of the project.

Probe-Induced Site-Selective Nanoscale Catalysis. SUKHMINE BAINS (University of California, Berkeley, Berkeley, CA 94720) STAN-ISLAUS S. WONG (Brookhaven National Laboratory, Upton, NY 11973).

Nanotechnology is the study of matter and phenomena at the nanometer scale. It is the anticipated wave of future manufacturing technology that will make products smaller, faster, less expensive, and more precise. It will enable fine control, on the molecular level, over reactivity, that will help to take molecular electronics beyond today's silicon-based device technology. As a first step, the objective of our current study has been to initiate a surface photocatalytic reaction in air, on the microscale utilizing the atomic force microscope (AFM). A nanoscale powder of a photocatalyst has been attached to an AFM tip and used to selectively degrade a synthetic textile dye, under the presence of UV radiation, within a spatially defined region. The degradation reaction was performed on a homogeneous surface of dye deposited on a glass substrate, and accelerated with the addition of H₂O₂. Confirmation of the reaction came through with the use of comparing optical microscopy images of the dye surface prior to and after UV irradiation. Optimization of the process is the focus of future efforts to establish conclusive validity of the results presented.

Gelcasting of Silicon Carbide and Silicon Carbide/Carbon Fiber Composites. JOSEPH MURPHY MURPHY (Lehigh University, Bethlehem, PA 18015) THOMAS LILLO (Idaho National Engineering & Environmental Laboratory, Idaho Falls, ID 83415).

Gelcasting is a relatively new forming technique that employs the use of a polymer cross-linking reaction to immobilize ceramic particles for the formation of complex-shaped parts. Combinations of various silicon carbide (SiC) powders, dispersants, and mediums were used in order to create slurries ranging from 30% - 50% solid loading, by volume. Trials were attempted with different amounts of powder additions and mill times. Slurries of SiC/carbon fiber composites were also made. Some composite slurries included dispersed chopped fibers while others

uni-directional, continuous fibers. A method, using methylcellulose and a pH of 11 as dispersants, to properly disperse the chopped fibers was developed. Water based slurries produced green bodies with densities of less the 50% of theoretical density and no significant increase in density was obtained from high temperature sintering (2200°C, 1 hr.). Isoproponal slurries yielded green densities ranging between 1.14 – 2.3 and sintered densities ranging from 1.0 – 2.1. The low green body densities are thought to be the cause for the lack of densification during sintering. Evidence points to porosity also being a reason for the lack of densification. The goal of this project was to have a sintered piece with a density of around 98% of SiC.

An Ultra High-Speed Detector for Intense Undulator Radiation. SEPEHR HOJJATI (*University of California, Berkeley, Berkeley, CA 94720*) DAVID ATTWOOD (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Synchrotron radiation is used for a wide range of scientific explorations. The basic idea is that when an electron accelerates it radiates. Being relativistic, the radiation is largely in the forward direction. While bending magnets, wigglers, and undulators are all magnetic structures used to generate synchrotron radiation, we are particularly interested in the bright and intense radiation produced by undulators. Such radiation can photo-emit some electrons from the surface of the sample. After following a circular path in the electric field of an electron energy analyzer, these electrons can be detected using an electron detector. The High-Speed Detector (HSD) at Lawrence Berkeley Laboratory has been developed in order to detect the electrons photo-emitted by undulator radiation. This project was part of the development of the software module, written in National Instrument's LabWindows environment, which enables the experimenter to set up and acquire data from the HSD for various types of experiments, particularly photoelectron spectroscopy. Furthermore, the software uses the Hierarchical Data Format, or HDF, a multi-object file format for sharing scientific data in a distributed environment, created at the National Center for Supercomputing Applications. Related experiments can be saved in one single HDF file, and numeric data (kinetic energy, angles, binding energy, etc.) can be then stored in the multidimensional arrays provided in the HDF library.

Magnetic Imaging Using the XM-1 Microscope. VICTOR CHAVEZ (*California State University Fresno, Fresno, CA 93710*) GREG DENBEAUX (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*). The XM-1 microscope at the Lawrence Berkeley National Laboratory can be used in several ways to obtain a high-resolution image of any sample. We know that the beam provided by the Advanced Light Source is in a plane parallel to the microscope. In order to get the highest intensity we would need to be at the center of the beam. But because we also want a high circular polarization, we actually need to be 2mm above the plane, which will give us a good combination of both intensity and circular polarization. After conducting several tests, we concluded that the XM-1 Microscope is 1.1mm above the plane. We have also taken several other images of magnetic activity using the XM-1. Co for example is a good sample to use when trying to find the best contrast I was also able to use the XM-1 to view magnetic writings. We set up a mechanism using a magnetic writing bit from a floppy disk drive connected to a wave generator. This gave the bit enough current to produce magnetic writings on a magnetic media. In this case we used a regular floppy disk. Our results showed that as we change the frequency from .5Hz to 1Hz and then to 2Hz at .25V, we see a change in the space between the magnetic writings. This can become very useful in these times. If we could pattern this on a small scale we would be able to save more data onto our hard drives, thus giving anyone an advantage in the computer market.

Pore Network Imaging Using the Focused Ion Beam and Image J 1.29v. THOMAS BARCENAS (*California State University-Fresno, Fresno, CA 93230*) LIVIU TOMITSA. PH.D (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Low oil recovery is due in part to inaccurate understanding of pore transport mechanisms of complex rock, of high of economic value, such as diatomite. Although scanning electron microscopy can provide indications of the pore 3-D structure, the absence of knowing the actual architecture of submicron rocks and their pore throat interconnectivities, and how they function under stress, causes the loss of oil recovery and ultimately, land subsidence. When using secondary recovery techniques for extracting oil, the preciseness of properly modeling the imbibition characteristics of diatomite is fundamental to recovery efficiency. In this project, the Focused Ion Beam apparatus was used to address these issues. Instead of the indirect inferring of the 3-D pore structure from traditional SEM images, the FIB method enables consistently accurate shaving of the sample surface followed by secondary ion beam image scanning. The shaving is accomplished by sputtering gallium electrons

(Ga+) across the surface, with energies of up to 30kV, and currents between 150-20,000 pA. The 2-D images, at thin as 0.01 microns, that are created, are then optimized for contrast using the imaging software Image J® 1.29v. and human depth of field visioning. After optimization, the images are thresholded, then binarized, aligned, and stacked to form a 3-D image. From these stacks more accurate extrapolations for algorithmic calculations can be made, yielding a more precise pore network schematic. Future work with this technology involves the use of thousands of these pore systems. A cold stage attached to the FIB will be used to image fluids in the pores. The chilling (immobilizing) of a saturated, oil-containing sample will enable the imaging of the fluid in contact with the pore walls. Thus, the contact angles can be determined in situ. This knowledge as well as other information applicable to NMR logs calibrations could be used to adjust existing sites being recovered.

Synthesis and Characterization of Fast, Bright IIb-VI semiconductor scintillator, ZnO. CHRISTOPHER HILL (*Alfred University, Alfred, NY 14802*) STEPHEN DERENZO (*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*).

Current research in semiconductor scintillators revolves around the characterization of luminescent materials with fast, bright emission. Short decay times, >1 ns, are a requirement in the medical imaging field for increasing sensitivity of Positron Emission Tomography. Other applications involve the use of Heavy-atom scintillators for improved gamma ray detection. Semiconductor scintillators such as Gallium doped ZnO and Indium doped CdS produce extremely fast emission, but light output is diminished when a significant concentration of holes are trapped on thermally activated nonradiative centers, possibly Zinc Vacancies. ZnO:Zn, a current commercial phosphor, produces extremely intense luminescence at room temperature, albeit slow, overcoming the influence of nonradiative centers. Controversy still exists over the exact defect species associated with the intense green fluorescence from ZnO:Zn. The paradigm exists for doubly doping ZnO with Gallium and another shallow acceptor, under a Zinc atmosphere to control the detracting effect of Zinc vacancies. CdS would present an analogous system and is being explored concurrently with ZnO.

Conducting and Optical Properties of Transparent Conducting Indium-Doped Zinc Oxide Thin Films by Sol-Gel. SUSAN HUANG (*SUNY Albany, Albany, NY 12222*) TANYA KAYDANOVA (*National Renewable Energy Laboratory, Golden, CO 89401*). Transparent conducting oxides were successfully prepared from mixed zinc nitrate hexahydrate and indium nitrate hydrate solutions in ethylene glycol using sol-gel technique. The In content in the film was varied (0,2,10,20,40,75 and 100 at %). Films were prepared by spin coating of the liquid precursors followed by thermal decomposition at 400°C after each layer. According to X-ray diffraction (XRD) measurements the pure ZnO and pure InO films (0 and at 100% In) were crystalline as-deposited. The crystallinity was suppressed in mixed compositions such that the films with compositions between 10 and 75 at % were completely amorphous. All the films were transparent with the transmission cut-off frequency near 400 nm, which is characteristic of TCO materials. All as-deposited films were conductive with 0 and 100 at % indium having the lowest resistivities. The resistivity of all compositions were improved by post-deposition reducing anneal in pure Ar at 300°C. The lowest resistivity obtained (0.2 Wcm for the pure ZnO after Ar anneal) was two-orders of magnitude higher than reported in the literature for the same composition which was attributed to the low processing temperature. The resistivities of as-deposited and annealed in Ar films were increased by consequent air anneal at 300°C.

Electrodeposition and Testing of Superconductor Bi-2212 Oxide Thin Layer on Lanthanum Aluminate and Silver. MARK WEHRENBURG (*University of Washington, Seattle, WA 98195*) RAGHU BHATTACHARYA (*National Renewable Energy Laboratory, Golden, CO 89401*).

Superconducting materials have the potential to vastly improve electrical efficiency and many modern technologies such as high current capacity power cables, magnetic resonance imaging (MRI) equipment, and magnetically levitated trains. For this to be realized, however, there must be improvements made to the composition of superconductor materials that will improve its current density (J_c), capacity in strong magnetic fields. Our purpose is to vary some of the parameters of the thin film making procedure in order to achieve a higher current density. Bi nitrate, Sr nitrate, Ca nitrate, and Cu nitrate are dissolved in Dimethyl Sulfoxide (DMSO) or water solvent and Bi, Sr, Ca, and Cu are electro-deposited onto an Ag coated Lanthanum Aluminate (LAO) or pure Ag foil substrate. The resulting thin films undergo an annealing process to form the desirable $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2$ (Bi-2212), and their superconductivity properties are measured. This report primarily concerns experimentation with different ED chemical bath compositions in order to deposit a

BSCCO thin layer with high J_c capacity in a strong magnetic field. Many difficulties were encountered in depositing the superconducting thin layer, including: patchy deposition layers, thickness gradient along the substrate, and proportionality gradient along the substrate.

Properties of Multi-Layer Pairing in Thin Film CdO-SnO₂ Produced by Chemical Vapor Deposition. MELINDA SCHROEDER (CU Boulder, Boulder, CO 80309) XIAONAN LI (National Renewable Energy Laboratory, Golden, CO 89401).

The purpose of this investigation was to determine whether multi-layer transparent conducting oxide (TCO) structures consisting of alternating layer pairs of tin oxide (SnO₂) and cadmium oxide (CdO) would yield Cd-Sn-O compound structures with favorable optical and electrical properties. The individual layers of SnO₂ and CdO film were deposited at different temperatures. Using a combinatorial synthesis approach, the CdO layer thickness continuously decreased along the flow direction of the reaction gas while the SnO₂ layer thickness remained constant. As a result, the CdO/SnO₂ ratio should have decreased and the optical and electrical properties of the multi-layer structures should have varied along the flow direction. As the composition varied, cadmium stannate (Cd₂SnO₄) spinel structure may also have formed. The total thickness of the multi-layer structures was measured with a stylus profilometer (Dektak3) and the individual pair layer thickness was determined by dividing the total multi-layer structure thickness by the number of layer pairs. The electrical properties (carrier concentration, resistivity, and mobility) of the multi-layer structures were analyzed with a Bio-Rad HL5500 Hall system. A Cary spectrophotometer was used to determine the transmittance, reflectance, and absorption spectrum of the multi-layer structures in wavelengths ranging from 250 nm to 2000 nm. Optical bandgap values were attained with the measured transmittance and reflectance data. X-ray diffraction (XRD) was used to determine the presence of crystalline structures and lattice constants. Two samples were studied: a bi-layer (one pair) sample and a multi-layer pair sample. Individual layer pair thickness decreased along the sample positions in both samples. Electrical properties were less desirable in the multi-layer sample than the bi-layer due to differences in layer pair thickness. Optical properties were better in the multi-layer sample and were not affected by layer pair thickness. The bi-layer sample had a combination of CdO and SnO₂ crystalline structures while the multi-layer sample had a distinct CdO crystalline structure with the presence of a structural anomaly. This anomaly prompted a study of the annealed section of the multi-layer sample. Analysis of the annealed section resulted in the discovery of a Cd₂SnO₄ spinel structure. Further analysis of other annealed layers may show improved TCO characteristics.

Single-Wall Carbon Nanotube Growth in a Volumetrically Confined Arc-Discharge System. KALE FRANZ (Colorado School of Mines, Golden, CO 80401) MICHAEL HEBEN (National Renewable Energy Laboratory, Golden, CO 89401).

Carbon nanotubes hold significant promise for a vast number of materials applications due to their unique mechanical, electrical, and gas storage properties. Although single-wall carbon nanotubes (SWNTs) have been synthesized since 1993 by the arc-discharge method, and numerous other synthesis methods have been developed, no synthesis method has yet produced 100% pure carbon nanotubes. Instead, a significant amount of amorphous carbon, nanocrystalline graphite, graphite, and metal catalyst a necessary ingredient for SWNT growth are present as impurities in the raw soot produced in the SWNT synthesis process. While the arc-discharge synthesis method was the first to produce SWNTs, it also produces more impure raw soot in comparison to the laser vaporization method. The more recently developed laser vaporization method has produced the purest raw soot to date but is a slower method of production. Geometry and thermal gradient are significantly different in the traditional arc-discharge systems and laser vaporization systems. We report that, by incorporating some of the characteristics inherent to a laser-vaporization system into an arc-discharge system, improvement in the yield of SWNT raw soot may be achieved. This is accomplished by confining the arc within a 50 mm diameter quartz tube, similar to the laser vaporization system. We find through transmission electron microscopy and Raman spectroscopy that SWNTs are made in significant numbers in this confined arc-discharge system, comparable to laser vaporization synthesized material. Further study is, however, required to prove reproducibility and attain an exact value for the purity of the produced raw soot.

The Characterization of the n-GaN/P2 Semiconductor for Direct Water Splitting. KATHRYN LEE (Miami University of Ohio, Oxford, OH 45056) JOHN TURNER (National Renewable Energy Laboratory, Golden, CO 89401).

Hydrogen has become a leading contender as an energy carrier for renewable energy. In order for it to be a cost effective, renewable and

practical fuel, we must find an efficient and environmentally friendly means of isolating hydrogen on a large scale. Currently, one of the most promising sources is water. Direct water splitting is one possibility. Direct water splitting uses photoelectrochemical processes to separate water into its hydrogen and oxygen components. This system consists of a semiconductor electrode which absorbs solar energy and produces a photocurrent. When immersed in water with a counter electrode to form a complete circuit, this photocurrent can split water, producing hydrogen and oxygen. The semiconductor material that we were researching for this purpose was n-type GaInP₂. In order for GaInP₂ to function in a direct water splitting process, however, the band edges and Fermi level must be shifted so that they overlap the water redox potentials. We treated the semiconductor surface with four different porphyrins that had been shown to successfully shift the band edges of the p-type GaInP₂ semiconductor to water splitting range. The porphyrins seemed to shift the band edges in the right direction after one hour, but not into water splitting range. After longer treatment, the band edges shifted in the opposite direction, becoming even more negative than without treatment. The porphyrin treatment also increased the doping density of the n-type, by some method that remains to be explained. Therefore, this material has yet to be modified for use in direct water splitting system.

AFM Surface Characterization of Thermal Grain Boundary Grooving on Rolling Assisted Biaxially Textured Substrates. RICHARD KINCH (University of the Sacred Heart, San Juan, PR 00914-0383) AMIT GOYAL (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The use of rolling assisted biaxially textured substrates (RABiTS) to produce high-temperature superconducting tapes is now a well-developed process. Several companies worldwide are attempting to scale this process up. Superconducting tapes are envisioned to have numerous applications in the electric power industry (Cables, transformers, motors, generators, etc), the medical industry (MRI, NMR) as well as in many other areas. A key component of the RABiTS substrate is a biaxially textured metal substrate with a cube texture. Typically high annealing temperatures are necessary to form a complete cube texture, which result in grain boundary grooving at all the boundaries present in the sample. Also, since each subsequent layer, i.e. the buffer layers and the superconducting layer, is deposited epitaxially on the metal substrate, the pattern of thermal grooves present on the substrate is also reflected on these layers. It is of interest to determine if the groove profiles are modified in a fully buffered substrate from that in the bare metal substrate; therefore, Atomic Force Microscopy (AFM) was used to characterize the grain boundary groove profiles of both a bare metal sample and a fully buffered sample. Thermal groove depth, groove width, and dihedral angle, formed at the root of the grooves, were characterized. These measurements were then classified as grain boundary grooves surrounding small grains or large grains. This distinction was done since higher angle misorientation surround the smaller grains. It was noted that in both the bare metal and the fully buffered sample the grain boundary grooves surrounding small grains were deeper, wider, and had smaller dihedral angles. There was also an appreciable difference for the results obtained from the fully buffered sample when compared to the bare metal sample. These results show that epitaxial deposition of the buffer layers indeed modifies the thermal grooving present in the RABiTS metal substrate, reducing the depth and width of these thermal grooves and increasing their dihedral angle.

Characterization of Electromagnetic Properties in YBCO Films on Rolling-Assisted Biaxially Textured Substrates. CARL HIPPER (Embry-Riddle Aeronautical University, Daytona Beach, FL 32114) PATRICK MARTIN (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The electromagnetic properties in YBa₂Cu₃O₇ (YBCO) superconducting films deposited on Rolling-Assisted Biaxially Textured Substrates (RABiTS) were investigated. Buffer layers consisting of Y₂O₃/YSZ/CeO₂ were deposited on a NiW tape to prevent the reaction between the YBCO layer and the Ni. Electron-beam co-evaporation of Yttrium, Barium Fluoride, and Copper was then used to deposit the YBCO precursor onto the substrates. A heat treatment was then performed to convert the precursor into the epitaxial YBCO superconducting layer (on the order of one micron in thickness). The electromagnetic properties investigated were critical current at 77-kelvin (I_{c77}) both in zero field and in the presence of various magnetic fields, the angular dependence of these fields on the I_{c77} of the superconducting tapes, and the effects on the tape's I_{c77} after several thermal cycles (77-298K). The measurements were all taken using an apparatus consisting of an electromagnet (with a maximum field of 1.5 tesla), a liquid nitrogen dewar capable of being set at various angles with respect to an applied magnetic field, and a four-point probe (two current leads, two voltage contacts) connected to a digital voltmeter. The results showed how stronger magnetic fields reduced the I_{c77} in the YBCO tape. This was expected because

the magnetic fields break up the Cooper pairs (paired electrons) that are essential to superconductivity. The YBCO tapes show an angular dependence of applied magnetic field on the Ic77 because of the microstructural orientation of the YBCO. The thermal cycle test showed the relative endurance of the YBCO tapes.

Computer controlled measurement of electrical conductivity in high-temperature ion-transport membranes. WILLIAM MICHIE (Howard Community College, Columbia, MD 21029) SCOTT A. SPEAKMAN (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Current ion transport membranes, such as proton conductors, have two undesirable deficiencies. They are either prone to chemical attack in their operating environment or they have poor ionic conductivity. Ion conducting LaYO_3 has a perovskite crystalline structure while $\text{La}_2\text{Zr}_2\text{O}_7$ has a pyrochlore structure. Combining these materials creates a network of phase boundaries between the structures that may increase ion transport. An essential step in evaluating $(\text{LaYO}_3)_{1-x}(\text{LaZrO}_3)_x$ mixed-conducting ceramics is the measurement of the electrical conductivity, which includes both electronic and ionic components. For ion-transport applications, conductivity should be measured over a range of 400°C through 1100°C. An instrument for measuring the conductivity over the necessary temperature range has been built. This instrument uses the 'van der Pauw' method for determining conductivity so that irregularities in the geometry of the sample do not adversely affect the accuracy of the measurement. A system for temperature control, data collection, and analysis was developed using LabVIEW® software. The software allows measurements to be automatically collected over an extended range of time and temperature. The program takes the necessary measurements and then calculates the subsequent conductivity. The accuracy of the computation was verified by direct comparison of the same data analyzed in an Excel® spreadsheet. Data were collected from a known standard and compared against published values to evaluate the accuracy of the instrument. Subsequently, the $(\text{LaYO}_3)_{1-x}(\text{LaZrO}_3)_x$ system was evaluated. This work provides an important component for ongoing research to identify superior ion conducting materials.

Effect of the Non-Parallelism and Roughness of the samples on Elastic Moduli Determined using Resonant Ultrasound Spectroscopy and Impulse Excitation. BRYAN SEARS (Eastern Arizona College, Thatcher, AZ 85552) MILADIN RADOVIC (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Resonant Ultrasound Spectroscopy (RUS) and Impulse Excitation (IE) are one of the most precise techniques for determination of the elastic moduli of solids. The precision of the RUS and IE strongly depends on the precision of the input data such as dimensions and weight of the samples. Despite this little is known about the sensitivity of RUS and IE on the deviation from ideal geometrical shape and roughness of the sample. To analyze effect of roughness and deviation from ideal geometrical shape of the sample on elastic moduli determined by RUS two groups of glass and steel discs were examined. The first group of examined steel and glass samples consist of the samples that were ground using 80-500 grit sandpapers to produce different roughness of the samples surfaces with average roughness determined by a profilometer. The second group of examined steel and glass samples consist of the samples that were ground to different angles (from 0-1 degrees) to produce different deviation from surface parallelism. It was determined that roughness does not significantly affect the precision of RUS up to the measured average roughness of 0.80 mm. The results from the tests on the samples that had non-ideal geometry showed that even slight deviations in ideal geometry have a huge affect on RUS precision for example a steel sample with a 1 degree angle caused a 14% decrease in the moduli of the solid. Care should be taken when using RUS in determining elastic moduli to ensure the ideal geometry of a sample and thus guarantee accurate results.

Evaluation of Friction Stir Processing for Surface Modification of Cast Aluminum Alloys. TYLER ENGSTROM (South Dakota School of Mines and Technology, Rapid City, SD 57701) DAVID, S.A. (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Friction stir processing (FSP), a derivative of friction stir welding (FSW), is being investigated as a potentially useful technique for surface modification of aluminum alloys. Materials employed for this research were common sand and permanent mold casting alloys A319 and A356. Ductility of as-cast material is very low. Microstructures of these metals consist of Al solid solution dendrites along with coarse silicon and intermetallic phases. Shrinkage porosity is also prevalent. Initial experiments involved optimization of process parameters through use of a modified Rosenthal heat generation model. Friction stir processed surface layers were then produced on plates of both alloys by making multiple overlapping passes with a conventional FSW tool. Microstructures of the FSP zones were characterized and specimens machined

from the plates for mechanical testing. Results show that FSP closed shrinkage porosity and homogenized as-cast microstructures by breaking up and evenly dispersing script phases. Hardness was increased in the stir zones while soft spots were eliminated. Tensile tests showed that FSP increased ductility in surface layers of A319 and A356 by 1410% and 565%, respectively. Due to these improvements in as-cast surfaces, FSP may reduce the risk of fatigue failure in A319 and A356 components.

High Density Infrared Surface Treatment of Ceramic Materials. HUGHES CRAFT (North Carolina State University, Raleigh, NC 27607) TERRY TIEGS (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

High Density Infrared (HDI) is a new technology being investigated for the treatment of ceramic surfaces to alter them physically and chemically. HDI produces high power densities (up to 3.5 kW/cm² at the ORNL facility) using a controlled plasma in a quartz lamp. The technology has advantages over existing laser melting technology, including a larger coverage area and the ability to process large surfaces in a relatively short time. Both metals and ceramics were treated using HDI. Commercial refractory bricks of aluminosilicates and magnesium oxide (MgO) were treated as-received in an effort to improve the wear properties of the surface and reduce surface porosity. To improve the corrosion resistance of the refractory bricks, they were also coated with approximately 100 mm of MgO, alumina (Al_2O_3), spinel (MgAl_2O_4) or yttria (Y_2O_3). The powder slurries were applied using the overall weight gain to estimate the thickness of the coating. In addition to the refractory bricks, applicability of the HDI process to wear-resistant carbide-based coatings on iron-based materials was investigated. Onto substrates of 4140 steel, D2 tool steel, and cast iron, coatings of WC-Co, WC-Ni, WC Ni₃Al, and TiC-Ni₃Al were applied. These coatings were applied, in slurry form, via an aerosol spray process. Optical characterization of the refractory samples showed the formation of a dense surface layer. The samples were also tested in a variety of ways. To determine their resistance to corrosion, the aluminosilicate refractory bricks were immersed in molten glass at 1400 OC for 100 hours, and the treated MgO bricks were immersed in a molten mixture of iron, chromium, and nickel at 1400 OC for 100 hours. The molten glass test showed that the treated surfaces provide an effective barrier for corrosion; the treated surfaces remained intact while the other sides showed significant degradation. Results from the MgO samples tested in molten metal are pending. X-Ray diffraction data on the MgO samples shows that HDI can be used to alter surface chemistry. On the samples with an alumina coating applied, the result after HDI treatment is a coating consisting predominantly of spinel. Optical microscopy and Vickers hardness testing of the carbide-based samples indicates some porosity in the coatings. Remaining work includes further characterization and wear testing of the carbide samples.

Investigation of Microtexture in Al 6061 Friction Stir Weld with Three Dimensional X-Ray Microscopy. JAMES LEATHERS (University of Texas El Paso, El Paso, TX 79968) GENE ICE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Friction Stir Welds (FSWs) are made by clamping the two parts to be joined to a rigid backing plate. A cylindrical-shouldered tool with a threaded pin is rapidly rotated and advanced along the weld line slowly. When the shoulder of the pin touches the work piece, frictional heat is generated causing severe deformation. Recrystallized fine grains with no porosity are formed in the weld region. The flow of materials is extremely complex and high textural heterogeneity is expected. In order to characterize the plastic flow, quantitative characterization of the crystallographic microtextures is needed. The present experiment determines the variation in local orientations in two Al 6061 FSWs using white beam Laue diffraction with X-ray microbeam of submicron resolution in three dimensions non-destructively. Depth resolved Laue patterns were obtained by differential aperture depth profiling. Variations in grain orientations with respect to the weld direction, the thickness direction, and the advancing side direction were determined by indexing the Laue patterns. The orientation of grain [100] directions inside the region that rotates with the pin ('carousel') on the retreating side are highly oriented with respect the thickness direction (TD). As movement away from the pin occurs, the grains have started to grow (2-4 microns) but still maintain the same orientation. A similar characterization can be made for the advancing side indicating that this region is dominated by the rotational rather than the advancing movement of the pin which would show an asymmetry with respect to the weld direction. Additionally, deviatoric strain was measured as a function of depth into grains at various locations around the weld. From the Laue patterns examined, the various spots show no elongation so there has evidently been sufficient annealing for dislocations to form subgrain walls. Each subgrain, however, will diffract in a slightly different direction indicating the misorienta-

tion between subgrains. These misorientations are indicative of plastic strain. Within the carousel region the strain is two orders of magnitude lower than in the weld path. It is thought that dynamic recrystallization in the carousel removes the defects nearly as quickly as they are formed.

Investigation of Microtexture in Al 6061 Friction Stir Weld with Three Dimensional X-Ray Microscopy. CHRISTIAN SCHMIDT (El Paso Community College, El Paso, TX 79903) GENE ICE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Investigation of Microtexture in Al 6061 Friction Stir Weld with Three Dimensional X-Ray Microscopy Friction Stir Welds (FSWs) are made by clamping the two parts to be joined to a rigid backing plate. A cylindrical-shouldered tool with a threaded pin is rapidly rotated and advanced along the weld line slowly. When the shoulder of the pin touches the work piece, frictional heat is generated causing severe deformation. Recrystallized fine grains with no porosity are formed in the weld region. The flow of materials is extremely complex and high textural heterogeneity is expected. In order to characterize the plastic flow, quantitative characterization of the crystallographic microtextures is needed. The present experiment determines the variation in local orientations in two Al 6061 FSWs using white beam Laue diffraction with X-ray microbeam of submicron resolution in three dimensions non-destructively. Depth resolved Laue patterns were obtained by differential aperture depth profiling. Variations in grain orientations with respect to the weld direction, the thickness direction, and the advancing side direction were determined by indexing the Laue patterns. Highly oriented grains with [110] parallel to the sample thickness were found. The grain orientation in the advancing side of the weld is opposite to that in the retreating side. Correlation between the microtexture and the FSW parameters is made

Lanthanum zirconate buffer layers deposited on biaxially textured Ni-3% W alloy substrates using metal organic decomposition for Coated-Conductors. STEVEN SCRUGGS (University of Houston, Houston, TX 77204) M. PARANS PARANTHAMAN (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Second generation coated conductors, which consist of a film of superconducting material deposited on a buffered flexible metal substrate, provide a promising solution for various high temperature superconductor applications. The rolling assisted biaxially textured substrate (RABiTS) approach, which was developed at ORNL, involves cold rolling and annealing of nickel or a nickel based alloy to produce cube texture (i.e. each grain is oriented with its (100) planes nearly parallel to the sheet surface and the [001] direction is nearly parallel to the rolling direction). Since diffusion of the metal substrate into the superconducting layer causes suppression in the transition temperature (T_c) and critical current density (J_c), buffer layers are used to provide a chemical barrier between the metal and the superconductor. The buffers are grown epitaxially on the substrate, thus providing a template for highly oriented nucleation and growth of the superconductor, which is necessary for high current densities. Vacuum deposition approaches currently being used for buffer layer processing are expensive and slow; consequently, much work is being done to develop an all-solution, non-vacuum route to scale up coated conductor processing. This study focuses on providing a stable, water insensitive precursor solution for use in a non-vacuum deposition process. Lanthanum zirconate buffer layers have been deposited by spin coating on biaxially textured Ni-3% W substrates using the metal organic decomposition process. The solution precursor was prepared by dissolving 2,4-pentanedionates of zirconium and lanthanum in methanol and glacial acetic acid. The films were annealed at 1100°C for 30 minutes under 4% H₂-Ar gas flow and the coating and annealing process was repeated several times to obtain thicker films. Texture analysis of the buffer shows full-width-at-half-maximum (FWHM) values for out-of-plane and in-plane alignments to be 8.35° and 9.42° respectively. Pole figure analysis indicates a single cube-on-cube texture while SEM micrographs reveal a dense, continuous, and crack-free buffer layer. Atomic Force Microscopy indicates a surface roughness of approximately 2 nm for the buffer which is suitable for further deposition of buffer layers or the superconducting layer. These results offer the potential for scale-up manufacturing of coated conductors with high current density using an all solution deposition approach.

Material Characteristics of Hydrogen Fuel Cell Electrolytes. AARON FERBER (University of Tennessee, Knoxville, TN 37996) ANDREW A. WERESZCZAK (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Solid oxide fuel cells (SOFC) are energy conversion devices that electrochemically combine a gaseous fuel (hydrogen or methane) and an oxidant (O₂ gas) via an ion conducting electrolyte thereby generating electricity and heat. SOFCs provide a more efficient and cleaner method of combustion than present day methods. To generate sufficient

voltage, small, individual fuel cells must be stacked and interconnected with each other and also heated to high temperatures (circa 1000°C). In addition to maintaining its role as an O₂ conductor, the electrolyte must also exhibit mechanical reliability as reflected by the mechanical strength. The primary objective of this project was to develop and verify a miniature biaxial test method to measure strength of a yttrium-stabilized zirconium oxide (Y-ZrO₂) electrolyte. The secondary objective was to investigate the effect specimen size and test geometry have on the statistical (Weibull) parameters, which describe the distribution of strengths typical of brittle ceramic materials. The ZrO₂ specimens were fabricated by laminating unfired, tape cast layers of 8Y zirconium tape into disc shaped specimens with a diameter of approximately 18 mm. Each layer was approximately 0.250 mm thick. Laminating was preformed by applying a thin coat of solvent/binder mixture to each tape interface, and pressed using a pressure of 10,000 pounds for 3 minutes. The disks were sintered at 1350°C for 8 hours in air, producing a normal relative density of 98%. Three variations in thickness were considered by testing specimens composed of single, double, and four layers of the tape, which exhibited average thickness 0.21 mm, 0.39 mm, and 0.82 mm respectively. All specimens had an average diameter of 17.2 mm. The specimens were tested at room temperature using a biaxial flexure test involving both ball-on-ring and ring-on-ring fixturing. The strength of the Y-ZrO₂ was found to decrease with increasing effective volume, which was calculated from a computer program written by the author. Although the Weibull modulus also decreased slightly from 8 to 6, the differences were not statistically significant for a 95% confidence interval.

Nb-1Zr Stress Analysis for Space Reactor Applications. ANDREW NELSON (University of Wisconsin - Madison, Madison, WI 53706) LANCE SNEAD (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Nb-1Zr is a refractory alloy that possesses the performance characteristics needed for operation in high-temperature, high-stress environments compounded by exposure to considerable neutron fluences. Past and current materials research has established an acceptable temperature-stress design window for Nb-1Zr. Embrittlement at temperatures below 800K provides the lower temperature boundary, and the upper limit is governed by the 100000 hour creep rupture stress curve to a maximum of 1500K. The design stress ceiling is specified as 1/3 the Ultimate Tensile Strength at intermediate (< 1100K) temperatures and the 100000 hour creep rupture stress at high temperatures. Each reactor design is subject to different operating conditions but when analyzed the Nb-1Zr primary clad stresses fell within acceptable limits for all three. The HPR cladding experiences the highest temperatures, but attains the lowest stresses of 5 MPa, well below the allowed limit of 20 MPa at 1350 K. The LMR reactor cladding will experience beginning of life stresses near 10 MPa and grow to nearly 20 MPa due to fission gas accumulation in the fuel pin plenum, but due to the lower operating temperature of approximately 1200 K this remains within the safe regime. Finally, the GCR design introduces a large axial temperature gradient along the length of each fuel pin and high pressure coolant to the analysis, causing stresses to catapult above 35 MPa. However, the lowest operating parameters of the proposed reactors (an entrance temperature of 900 K and exit of 1150 K) equate to a maximum design stress near 70 MPa such that the Nb-1Zr primary stresses again fall within the acceptable boundaries.

Proton conducting membranes for hydrogen separation. CLARK RITZ (Carleton College, Northfield, MN 55057) TIM ARMSTRONG (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Due to limitations in today's fossil fuels new energy sources must be found. One promising option is hydrogen, which is produced primarily by steam reforming of methane. This process results in a mixed gas stream composed of CO, CO₂, H₂, and H₂O, from which H₂ must be separated and purified before use in petroleum upgrading or for use in fuel cells. Separation of H₂ from the feed stream can be achieved with an ion transport membrane. Possible candidate membrane materials are ceramics with large defect volume, such as strontium doped lanthanum niobates. Powders with the compositions La_{1-x}Sr_xNbO₄, where x = 0.1 -> 0.4, were produced through glycine-nitrate combustion synthesis. Powders were calcined until single phase as determined by X-ray diffraction. Pellets were pressed from single phase compositions and were sintered. The goal of this project was to investigate new materials, optimize their composition for proton conductivity and characterize their other pertinent properties. X-ray and SEM analysis show that the La₂O₃-SrO-Nb₂O₅ system does not form a homogeneous single-phase material. Investigation of this system was terminated, and an investigation of the La₂O₃-SrO-Ta₂O₅ system was initiated.

Residual Stress Measurements of Cast Aluminum Engine Blocks Using X-Ray Diffraction. DAVID WIESNER (*University of Tennessee, Knoxville, TN 37916*) THOMAS R. WATKINS (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

The engine casting plant of Honda (Anna, OH) identified the development of residual stresses in their cast aluminum engine blocks to be due to differential cooling during processing. Concern for the presence of these stresses derives from the distortion of critical features caused during machining, which increases the difficulty of maintaining dimensional tolerances. This is particularly true for features that have close tolerances, such as bearing journals. In an effort to remove these residual stresses, the engine blocks are subjected to a T5 stress relief treatment prior to machining. The addition of this stress relief treatment has added complexity to the process, and the stress relief oven has become a major production volume-limiting step. Alternate stress relief cycles, capable of allowing greater throughput in the stress relief oven, would be beneficial in this regard. To achieve this objective, the residual stress in the engine block was mapped using X-ray diffraction, a fast and reliable technique for measuring residual stresses. The experimental work carried out at ORNL will facilitate understanding the process of residual stress relief treatment. Testing and data collection on as-cast and annealed engine blocks was completed using the large sample stress analyzer. Coordinate-mapping was used for radial and hoop stress measurements for automated testing. The collected data was generated for the aluminum (311) peak, using chrome radiation. Data analysis was performed using LabVIEW software that was developed for improved efficiency and quality of data analysis. As expected, analysis of the hoop stress results showed an overall reduction in compressive stresses and increased uniformity in the stress levels over the mapped surface with increase heat-treatment. The radial stress results, however, shifted from compressive to tensile with no change in uniformity with increasing heat treatment. This shift may be attributed to the complex geometry of the engine block resulting in the radial direction being constrained.

The Structural and Mechanical Properties of Materials for Solid Oxide Fuel Cells. LISA KRUEGER (*Oxnard College, Oxnard, CA 93041*) MILADIN RADOVIC (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Solid Oxide Fuel Cells (SOFC), as electrochemical devices that produce electrical energy, are being intensively investigated world-wide. At present, a typical SOFC consists of several multilayered stacks that are composed of a fully-dense electrolyte layer embedded between porous cathode and anode layers. Although the electrochemical properties of materials for SOFCs are well characterized, very little is known about their mechanical behavior. The main goal of this study is to learn more about the mechanical behavior of tape-cast Zirconia stabilized with 8mol% Yttria that is commonly used as a SOFC electrolyte, and 75mol% NiO/25mol% YSZ (NiO/YSZ) that is a precursor to Ni/YSZ anodes. In addition, the anode material was characterized after full reduction of NiO in hydrogen. The biaxial strength of the samples was determined by the ring-on-ring test while fracture toughness was determined by double-torsion testing. The electrolyte and anode samples of different porosity were characterized at ambient and elevated temperatures. It was found out that biaxial strength of YSZ Electrolyte decreases while biaxial strength of NiO-YSZ slightly increases with temperature. Results of biaxial testing also show that increase of porosity causes decrease in biaxial strength for both, NiO-YSZ and Ni-YSZ anode. After hydrogen reduction of NiO-YSZ to Ni-YSZ biaxial strength of anode decreases significantly, primarily because of the increase in porosity while fracture toughness increases significantly due to the change in fracture mechanism.

Thermal Effectiveness of Graphite Foam as a Heat Management Device. THOMAS BATTISTE (*University of Tennessee, Knoxville, TN 37916*) APRIL MCMILLAN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

High thermal conductivity graphite foams are being looked at for thermal applications in electronics. The objective of this study is to determine the effectiveness of 0.5 to 0.65 g/cc graphite foams as both heat spreaders and as heat sinks. Two different densities of foam plates (medium and high), three different heights of aluminum heat sinks (0.5 in, 1 in, 1.5 in), and two types of graphite foam heat sinks (0.5 in and 1in finned heights) were tested. A resistive heater was placed on an aluminum base plate with six thermocouples (TC) to simulate operational conditions; one TC was embedded in the base plate just under the heater, while another was embedded just over the heater. Four additional TCs were embedded, one in each corner of the base plate to measure heat spread. Using various voltages (0 - 60 Volts), temperature data were collected and analyzed. Initial testing showed a high thermal

resistance due to a lack of contact between the foam and the aluminum surfaces. There may also be an issue with the aluminum base plate not being able to conduct enough heat into the foam. This will be modified by plasma spraying a conductive material onto the contact surfaces of the foam, thus increasing its contact area. Then a direct placement of the foam to the heater will be performed. The last test that needs to be run is a test in which a series of thermocouples will be placed in a line from the center of the heater to the edge of the foam to measure the amount of heat spread across a billet of foam.

Cerium High Temperature Oxygen Generation and Cathode Evaluation. KEEGAN DUFF (*Portland Community College, Portland, OR 97280-0990*) KERRY D MEINHARDT (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The High Temperature Ceramic Oxygen Generator Cathode performance of $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-d}$, $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-d}$, and $(\text{La}_{0.8}\text{Sr}_{0.2})_{0.98}\text{MnO}_{3-d}$, supported on 130 micron $\text{Ce}_{0.8}\text{Sm}_{0.2}\text{O}_{3-d}$ electrolyte was tested over the range of 600-800°C. $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-d}$ yielded the highest performance of the three cathodes tested. The $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-d}$ was also evaluated at 600-750°C on anode supported 10 micron $\text{Ce}_{0.8}\text{Sm}_{0.2}\text{Fe}_{0.2}\text{O}_{3-d}$ electrolyte. The anode supported cell had significantly higher performance than the 130 micron electrolyte samples. The cathodes performance was evaluated using IV sweeps by changing the driving voltage and measuring the current. The cells were also analyzed using scanning electron microscope (SEM) to access porosity and microstructure.

Comparing Surfaces and Engineered Interfaces using Self-Assembled Monolayers (SAMs) and Injected SAMs silanes. MARK MORRIS (*Schenectady County Community College, Schenectady, NY 12302*) KEVIN SIMMONS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The objective of this study was to show a comparison between property changes by formation of a self-assembled monolayer on the surface of PPG synthetic precipitated silica, which is a technique developed at PNNL, and by adding the SAMs silane chemical directly into the mixing bowl. These coatings have the potential to greatly increase the bond strength and enhance other properties between the particle and the rubber matrix of a rubber compound. Tensile testing measured peak stress and elongation at break. The increase in tensile strength shows how well the polymer-filler interfacial adhesion is doing. The study used five different SAM systems with a sulfur cured styrene butadiene rubber (SBR) tire rubber formulation. The three propylsilanes were propyl triethoxysilane, allyl triethoxysilane and 3-mercaptopropyl triethoxysilane. Five combinations of silanes were used in this study. The application of the silanes were 100% propyl triethoxy silane (100% Alkyl); a 10/90 mixture of allyl and propyl triethoxy silanes (10% vinyl/90% alkyl); a 50/50 mixture of the allyl and propyl (50% vinyl/50% alkyl); a 10/90 mixture of 3-mercaptopropyl trimethoxysilane and propyl trimethoxysilane (10% mercaptan/90% alkyl) and lastly a 50/50 3-mercaptopropyl and propylsilanes (50% mercaptan/alkyl). The data not only shows improvement with SAMs, the peak stress data (ultimate strength) shows that by changing the amount of silane content can change the physical properties

Comparisons of Polymer Systems for Lamination of Clear Panels. ASHLEIGH COOPER (*University of Washington, Seattle, WA 98195*) KEVIN L. SIMMONS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Polymers have been used as interlayers in laminating systems to manipulate and influence properties. Typically, polymeric sheets have been used to bond substrates together. It is within the scope of this project to investigate the feasibility of laminating using free flowing resin systems. Various epoxy, polyurethane, silicone, polyester, and UV curable acrylate systems were investigated. Resins with applicable material properties were used to fabricate clear panel laminates for testing. The testing completed in time for this paper is limited to the UV-visible-infrared light transmission, however it is the intent of the project to continue testing to include impact strength, bond strength between panel and polymer, sound transmission, along with weathering properties of the laminate. Overall, the work conducted thus far has proven the viability of this technique along with directing the investigation towards appropriate resin systems for industrial applications.

Growth and Characterization of Oxide Nanostructures. ADAM DIRKES (*University of Washington, Seattle, WA 98195*) SUNTHAR-AMPILLAI THEVUTHASAN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Because the catalytic behaviors of certain elements change according to their size, the growth and characterization of oxide nanostructures provides useful knowledge for the development of more efficient fuel

cell technology and catalysts of environmentally harmful gas. The objective of this two-part study is to devise a process to create a catalyst in which precise size and density parameters are obtained and utilized to maximize efficiency of both oxygen ion transfer and catalytic properties. We use Molecular Beam Epitaxy (MBE) in an ultrahigh vacuum (UHV) system to disperse certain metals onto a variety of sample substrate materials. It is known that ceria (CeO_2), especially when doped with gadolinia (Gd_2O_3), transports oxygen ions very well [1]. In the first study, an yttria stabilized zirconia (YSZ) substrate is covered with a film of pure zirconia to insulate the ionic conductivity contribution from the YSZ substrate. Then ceria and zirconia films doped with gadolinia are alternately layered in different thickness configurations over the pure zirconia film. In doing this we are observing the influence of gadolinia through analysis of oxygen ionic conductivity to better understand the atomic and ionic transport processes in these nanostructured materials. Preliminary results show a higher conductivity with increasing layers of ceria and zirconia. It is also known that gold (Au) nanostructures bonded to titanium oxide (TiO_2) create a highly efficient catalyst in converting carbon monoxide (CO) to carbon dioxide (CO_2) [2]. In the second study, gold and titanium oxide clusters are grown on a substrate of highly ordered pyzolithic graphite (HOPG). So far, we have created a successful process of growing and annealing titanium oxide (titania) on HOPG to produce islands ~5 nm in diameter. Currently, we are devising a process in which gold approximately 3 nm in diameter is grown on the titania. These studies will help develop a greater understanding of the behavior of nano crystalline structures as opposed to the current understanding of bulk materials.

Investigation of Electrode Properties for a Reversible Solid Oxide Fuel Cell. KATHERINE MING (*Sacramento City College, Sacramento, CA 95864*) OLGA A. MARINA (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The purpose of this study was to investigate the ability of Solid Oxide Fuel Cell (SOFC) electrodes to operate reversibly as a fuel cell and an electrolyzer. Reversible SOFCs potentially can be used for hydrogen and electricity production. Porous platinum and nickel - yttria-stabilized zirconia (YSZ) electrodes were screen-printed and sintered onto dense YSZ electrolyte pellets. Electrode polarization resistances were measured while altering temperature and fuel gas partial pressures. Under the conditions studied, low hydrogen and high steam partial pressures and 700-900°C, nickel-YSZ and platinum did not appear to be efficient electrodes for reversible SOFCs. Platinum electrode exhibited high polarization losses. Nickel-YSZ electrode seemed to be unstable at high water partial pressures and degraded over 18 hours of testing.

Modeling of Kinetic and Thermodynamic Behavior of Oxide Formation during Stainless Steel Corrosion. DANIEL PARKS (*Whitman College, Walla Walla, WA 99362*) EDWARD SIMONEN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Intergranular stress-corrosion cracking, a type of cracking found in alloys, is characterized by the formation of stress cracks aided by electrochemical corrosion at grain boundaries. Crack propagation is heavily dependent on the passive salts and oxides that form on the surface of the crack as a result of the electrochemical corrosion processes. The conditions of formation for these salts and oxides are therefore of great interest. The internal PNNL program 'SChem', which is used to calculate the Ni_2 concentration in a stainless steel stress crack, was modified to conform to the slip-oxidation model of corrosion; a variety of calculations were conducted to characterize the kinetic behavior of the diffusion of ions within the crack. Using the concentration data generated by SChem, the commercial software application 'The Geochemist's Workbench' was used to create Pourbaix diagrams of the crack environment to predict the thermodynamic stability of chemical species within the crack. Predictions generated by this process will be helpful in understanding the passivation of the crack walls and tip.

Nanotips for Enhanced Electron Emission. CLAIRE MCQUERRY (*Gonzaga University, Spokane, WA 99258*) GLEN DUNHAM (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The current-voltage (I-V) characteristics of nanotip arrays of varying densities, defined by photolithography and wet-etched into n-type silicon wafers, were compared to the I-V characteristics for unetched silicon wafers. A method to improve tip sharpness by re-oxidation was also explored, and fabricated arrays were examined with SEM.

Photo-induced Phenomena in Arsenic Trisulfide. CONSTANCE FAY, RACHEL DIEKEN, HUGH BARNABY, PIERRE LUCAS, STEVE MACDONALD, and B. G. POTTER, JR. (*University of Arizona, Tucson, AZ, 85719*) S. K. SUNDARAM, BRADLEY R. JOHNSON, NORMAN C. ANHEIER, AND PAUL J. ALLEN (*Pacific Northwest National Laboratory, Richland, WA 99352*). Chalcogenide glasses (amorphous materials based on S, Se, or Te) are

highly transparent in the near to far infrared (1 μm to 20 μm). They are of great interest for optical imaging, chemical sensing, and communication devices at these wavelengths. These materials exhibit a high degree of photosensitivity such that localized changes can be made to the refractive index by exposing the glass to laser light at their absorption edge. Consequently, photonic structures can be made from these materials by direct laser writing. The present work investigated photo-induced phenomena in As_2S_3 chalcogenide glasses in bulk and thin film form in order to optimize the parameters needed to directly laser write photonic structures in this material. Experiments were done to determine the time and intensity dependent optical (photo-darkening) and structural (photo-expansion) response of As_2S_3 bulk glass and thin films. These were done using a HeNe laser (632.8 nm). The influence of material processing history on these photoresponses was also examined. Thin films were thermally evaporated in a vacuum coater, at two different crucible temperatures, using a temperature-controlled heater. In addition, the photo-response of annealed vs. unannealed thin films was studied. The optical properties and microstructure of bulk glass and thin film specimens were characterized using UV-Vis absorption spectroscopy, Raman spectroscopy, and X-ray diffraction (XRD). Photodarkening was evaluated by measuring transmitted power as a function of time during laser exposure. Optical profilometry, and scanning electron microscopy (SEM) were used for photoexpansion measurements on arrays of laser irradiated spots created at a given laser power with different exposure times. Photoinduced absorption change was evident in all samples; the rate of darkening and the magnitude of intensity change was directly related to laser power and the duration of exposure. Photoinduced physical changes in the bulk samples showed increased volume with longer exposure time and with higher exposure powers. The damage threshold for As_2S_3 was determined to be at a power density of 2.0 kW/cm² for all the tested samples. A power density of 1.9x10⁶ mW/cm² was required to achieve 50% relative change in photodarkening within 9.6 sec. This data directly supported efforts to create optimized laser written structures in As_2S_3 glass.

Separation & Fixation of Toxic Components in Salt Brines Using a Water-Based Process. CARRIE FRANKS (*University of Arizona, Tucson, AZ 85721*) ANH QUACH (*University of Arizona, Tucson, AZ 85721*) HARRY SMITH and GARY SMITH (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Efforts to implement new water quality standards, increase water reuse and reclamation, and minimize the cost of waste storage motivate the development of new processes for stabilizing waste water residuals that minimize waste volume, water content and the long-term environmental risk from related by products. This work explores the use of an aqueous-based emulsion process to create an epoxy/rubber matrix for separating and encapsulating waste components from salt laden, arsenic contaminated, amorphous iron hydrate sludges. Such sludges are generated from conventional water purification precipitation/adsorption processes, used to convert aqueous brine streams to semi-solid waste streams, such as ion exchange/membrane separation, and from other precipitative heavy metal removal operations. In this study, epoxy and polystyrene butadiene (PSB) rubber emulsions are mixed together and then combined with a surrogate sludge. The surrogate sludge consists of amorphous iron hydrate with 1 part arsenic fixed to the surface of the hydrate per 10 parts iron mixed with sodium nitrate and chloride salts and water. The resulting emulsion is cured and dried at 80°C to remove water. Microstructure characterization by electron microscopy confirms that the epoxy/PSB matrix surrounds and encapsulates the arsenic laden amorphous iron hydrate phase while allowing the salt to migrate to internal and external surfaces of the sample. Salt extraction studies indicate that the porous nature of the resulting matrix promotes the separation and removal of as much as 90% of the original salt content in only one hours time. Long term leaching studies based on the use of the infinite slab diffusion model reveal no evidence of iron migration or, by inference, arsenic migration, and demonstrate that the diffusion coefficients of the unextracted salt yield leachability indices within regulations for non-hazardous landfill disposal. Because salt is the most mobile species, it is inferred that arsenic leaches from the host material at an even slower rate, making the waste forms amenable to unregulated land disposal options. These result indicate that the environmentally-benign, water-based emulsion processing of epoxy/PSB polymeric hosts show great promise as a separation and fixation technology for treating brine streams from wastewater treatment facilities.

MEDICAL AND HEALTH SCIENCES

Chronic Oral Methylphenidate Usage in Rats. JASON-FLOR SANSANTE (State University of New York at Stony Brook, Stony Brook, NY 11790) PANAYOTIS THANOS (Brookhaven National Laboratory, Upton, NY 11973).

The psycho-stimulant methylphenidate (MP) is the most prescribed drug used in treating Attention Deficit Hyperactivity Disorder (ADHD). With an estimation of 3 million American children on the drug, MP usage has become a topic of controversy; the debate on MP usage is further emphasized due to lack of data examining the drug's long-term use. The effects of chronic oral MP, or Ritalin, usage are reported in this study. Young male rats were divided into three treatment groups: high dose at 2 mg/kg MP, low dose at 1mg/kg MP, and control (water). At two-week intervals for 28 weeks, rats were subjected to locomotor tests. Results show that locomotor differences occurred between saline and apomorphine treatments during the 28-week period: compared to baseline (saline) locomotor trials, the apomorphine trials yielded an increase in locomotor activity.

Developing methods to induce and detect biosynthesis of radiolabeled anandamide. SARA GONZALEZ (University of Scranton, Scranton, PA 18510) ANDREW GIFFORD (Brookhaven National Laboratory, Upton, NY 11973).

Anandamide (AEA), an endogenous compound that binds to the same receptors as 9-THC (the active compound in marijuana), interests researchers who hope to understand the way that the body produces the compound, which mimics 9-THC in function and perhaps in therapeutic value. Normally the compound's extremely short in-vivo half-life hinders investigation; thus, in this experiment mice genetically engineered to lack fatty acid amide hydrolase (FAAH), the enzyme responsible for the breakdown of AEA, were used in order to eliminate this challenge. Use of these 'knock-out' mice increased the time that AEA remained intact, facilitating research on this compound. A method was developed to radiolabel AEA by incubating live brain slices in 3H arachidonic acid (AA) and then inducing the release of AEA by incubating in depolarizing media. The brain slices were then homogenized, purified by centrifugation and simple extraction, and analyzed using high pressure liquid chromatography (HPLC). UV-detection and scintillation counters were used to confirm the presence and identity of radiolabeled AEA, which had been synthesized by the brain slices that had taken up the 3H AA during incubation. Thin Layer Chromatography (TLC) was used to verify the identity of AEA. This method of radiolabeling and analysis can be used to further investigate the biosynthesis and release of AEA.

Microbeam Radiation Therapy and its Potential in the Treatment of Gliomas. AMY FELDMAN (Valdosta State University, Valdosta, GA 31602) F. AVRAHAM DILMANIAN (Brookhaven National Laboratory, Upton, NY 11973).

Primary brain tumors affect over 40,000 Americans each year with malignant gliomas representing over 50% of these cases. With survival rates not improving over recent years, a new form of cancer therapy is needed. This is especially true for pediatric brain tumors, of which children under three years of age cannot be treated by radiation therapy. Microbeam Radiation Therapy (MRT) uses arrays of parallel, thin (<100 µm-wide) planar slices of synchrotron-generated X-rays of 50-150 keV energy. MRT spares normal tissues up to very high doses. This may be because the spacing between beams leaves bands of vascular endothelial cells unharmed in the normal tissue to regenerate, and repopulate the damaged endothelial cells. MRT also preferentially kills tumors. This may be because the tumor's vasculature is abnormal, and does not seem to be able to repair the microbeam damage. The current goal of the program is the study of the biological mechanisms underlying MRT effects, using immunohistochemistry. An important question during histological examination is to relate the observed effects to the position of MBs on the tissue section. Two separate experiments were conducted at the X17B1 beamline of the National Synchrotron Light Source (NSLS) with rats bearing intracranial 9L gliosarcoma (9LGS) tumors. The tumors were inoculated using 9LGS cell cultures. The rats were irradiated 14 days later with sparse microbeams at very high doses. They were euthanized at specified time points of: 1 hour, 3 hours, 8 hours, 2 days, 4 days, 1 week, 2 weeks, 1 month, and 2 months for histology. The brains were sectioned in 5 µm slices, placed on slides, and stained with hematoxylin and eosin (H&E), or hematoxylin only. The work was carried out in collaboration with scientists from University of Colorado Health Sciences Center, Denver. Histological and data analyses were performed on these slides. The goals were to verify the hypotheses that microbeams damage the tumor's vasculature but not the normal tissue's

blood vessels. Our experiment achieved its goal by finding evidence in support of both these hypotheses.

Mitogenic activity of FGF-2 and synthetic peptides. JASOHN GERLAK (Boston College, Chestnut Hill, Ma 02456) LOUIS PENA (Brookhaven National Laboratory, Upton, NY 11973).

One of the many biological functions of basic fibroblast growth factor, (bFGF a.k.a. FGF-2), a mitogenic cytokine, is the induction of cell proliferation through the mitogen-activated-protein-kinase (MAPK) signaling pathway. In order to deduce whether or not chemically produced analogs of FGF-2 behave in the same mitogenic fashion as the recombinantly produced FGF-2 protein, an assay involving the detection of phosphorylated MAPK (pMAPK) in stress-starved C3H10T1/2, mouse fibroblast cells, was performed; fifteen minutes after cells were treated with the FGF-2 and analog peptides designated to mimic the factor. Using untreated starved cells as a control, the relative amounts of pMAPK were compared to that in cells treated with recombinantly produced FGF-2 and chemically produced analogs of FGF-2. Result of the assay has shown that chemically produced analogs of FGF-2 not only trigger the phosphorylation of MAPK, inducing mitogenic activity, but the analogs do so more efficiently than recombinantly produced FGF-2.

Purification of Synthetic Cytokine Analogs. IVONNE CUMMINGS (Suffolk County Community College, Selden, NY 11784) LOUIS PEÑA (Brookhaven National Laboratory, Upton, NY 11973).

In the study of synthetic cytokine analogs responses, finding the proper conditions and method of purification are crucial. Reversed phase and affinity chromatography were used for the purification of various analogs of the cytokine basic fibroblast growth factor (bFGF, a.k.a. FGF-2). The reverse phase method gave less than 10% recovery where the affinity chromatography gave 10% or more. All different peptides have different affinity to heparin yielding different results in the recoveries.

The D3 Antagonist, SB-277011, and Morphine-Induced Conditioned Place. SANDRA SAINT VICTOR (State University of New York at Stony Brook, Stony Brook, NY 11790) ONARAE V. RICE (Brookhaven National Laboratory, Upton, NY 11973).

Dopamine has been found to be the cause of the 'reward' feeling attributed to many drug addictions. It has been suggested that the involvement of dopamine in morphine-induced place preference is mediated through D1 and D2 receptors but little information is known about the function of the D3 receptors. Conditioned place preference (CPP) is a procedure that is often used to test the effects of this 'reward' mechanism in correlation with an environmental cue. In this experiment, a reinstatement conditioned place preference paradigm was used to see whether or not time will diminish the affects of the morphine induced preference. Reinstatement of the positive place preference was tested by a prime injection of morphine. In addition, a D3 receptor antagonist, SB-277011 {trans-N-[4-[2-(6-cyano-1,2,3,4-tetrahydroisoquinolin-2-yl)ethyl]cyclohexyl]-4-quinolinecarboxamide}, was also used in correlation with the reinstatement and classic paradigm in order to examine whether or not this compound does in fact eliminate or reduce the established positive place preference. Rats were conditioned for four days with 45 min pairings of one chamber with morphine (10 mg/kg, intraperitoneally, i.p.) and the other chamber with saline. At the end of this phase the rats showed a positive place preference. The morphine induced preference was extinguished by pairing both chambers with saline for 45 min for four days. The animals continued to elicit a positive place preference for the morphine paired side after a prime injection of the drug (5 mg/kg) was administered. After administration of the D3 antagonist, SB-277011 (10mg/kg), a reduction in the elicited positive place preference was observed. Further investigation needs to be conducted in order to confirm the effectiveness of the SB-277011 antagonist.

The Effects of Chronic Ketamine on the Response to a Serotonergic Drug Challenge Using MicroPET and Microdialysis. LAUREL ECKE (Pomona College, Claremont, CA 91711) STEPHEN DEWEY (Brookhaven National Laboratory, Upton, NY 11973).

Ketamine has become well known for two main reasons: as a model for schizophrenia and as a recreational club drug commonly called Special K. Ketamine, an NMDA receptor antagonist, has wide-ranging effects including impact on not only glutamatergic neurotransmission but on dopaminergic and serotonergic neurotransmission as well. This investigation tested an animal's response to a fluoxetine (Prozac) challenge, a selective serotonin reuptake inhibitor (SSRI), before and after chronic ketamine treatment. It is important to look at the effects of antidepressants on cerebral function of schizophrenics because antidepressants are often used in combination with antipsychotics to treat schizophrenia. Animals were treated with ketamine by osmotic pumps implanted subcutaneously, which exposed the animals to a subanesthetic dose of 30 mg/kg/day of ketamine for 7 days. Microdialysis and microPET

were used to determine whether there was any change in brain function in response to ketamine and in response to a 20 mg/kg i.p. fluoxetine challenge prior to and following ketamine exposure. Microdialysis was used to measure change in extracellular serotonin levels in the striatum while microPET, using FDG as a radiotracer, measured change in glucose metabolism. Regions of interest (ROIs) were drawn over the left and right striatum, frontal cortex, parietal lobe, thalamus, temporal lobe, occipital cortex, and the cerebellum to observe which regions changed their rate of glucose metabolism. Using microdialysis, no change in extracellular serotonin was found in response to a fluoxetine challenge either prior to or following ketamine exposure. Using microPET, the rate of cerebral glucose metabolism dropped significantly 1 day following ketamine exposure and increased again slightly 1 week following ketamine exposure. Animals showed a higher rate of glucose metabolism in response to a fluoxetine challenge following ketamine exposure than prior to ketamine exposure. Thus a 7-day chronic exposure to ketamine causes a uniform decrease in glucose metabolism across the brain. Additionally, the central nervous system may respond differently to a serotonergic drug after having received ketamine. It is necessary to further investigate the effect of ketamine on the brain by performing additional experiments with a larger sample size. By researching ketamine, insight into the neurochemical changes that occur in the brains of ketamine abusers and schizophrenics can be achieved.

The Role of CB-1 Receptors in Alcohol Drinking. ELIAS DIMI-TRAKAKIS (SUNY Stony Brook, Stony Brook, NY 11790) PANAYIOTIS THANOS (Brookhaven National Laboratory, Upton, NY 11973). Cannabinoids are postulated to play a role in modulating the reinforcing effects of abused drugs including alcohol. Experiment 1 examined alcohol self-administration in cannabinoid CB1 receptor knockout (KO), heterozygous (HT) and wild-type (WT) mice in a two-bottle choice paradigm. Mice were trained in a limited 8-hour access / day to 10 % (v/v) ethanol versus water. After baseline drinking mice were treated (ip) with the CB1 antagonist SR 141716A (5 mg/kg). Data analysis consisted of % ethanol preference and ethanol intake (g/kg). Experiment 2 examined the CB1 WT and CB1 KO strains in a conditioned place preference (CPP) procedure (using a standard 3-compartment apparatus) between saline and 2 mg/kg ethanol. Percent time spent in each compartment was measured and compared across strain. Results indicated that the CB1 WT mice displayed significantly higher ethanol consumption compared to CB1 KO mice. Treatment with SR 141716A significantly attenuated ethanol intake in the WT and HT mice. Finally, CPP analysis revealed that the WT mice spent significantly more time in the ethanol-paired versus saline-paired compartment. No difference in CPP was observed in the KO mice. These data demonstrate that the cannabinoid CB1 receptor is an essential component of the molecular pathway determining alcohol consumption. This work was supported by the NIDA, DA06891-06. and the US Department of Energy DE-AC02-98CH10886.

The Role of Endogenous D2 Receptor Levels in Morphine Addiction. NAQI KHAN (Cornell University, Ithaca, NY 14853) S. JOHN GATLEY (Brookhaven National Laboratory, Upton, NY 11973). Dopamine is a neurotransmitter that has a wide array of effects on an individual's mental state. It is known to be vital in the regulation of motor skills as well as in substance abuse. This study examined D2 - a dopamine receptor found in the striatum of the brain. The impetus for investigating this receptor lies in the perception that it plays an influential role in drug addiction. It has been conjectured on the basis of human PET studies that low levels of endogenous D2 will heighten an individual's susceptibility to drug addiction. However, an alternative explanation of low D2 receptor levels in drug dependent individuals is that these levels are a consequence of drug abuse. To understand this phenomenon, the present study employed the paradigm of conditioned place preference (CPP). In CPP, individuals of an out-bred mouse strain are observed to spend time in environments where they had previously been exposed to a drug that is abused by humans. The drug of choice was morphine because it has been previously shown to generate a robust place preference in mice and is a prototypic abused drug in humans. The endogenous D2 levels were quantified using an in vivo binding study involving [3H]-RAC, a radioactive compound that binds to D2 receptors. The results showed a significant place preference for morphine following the conditioning procedure. Additionally, data from the binding analysis agreed with previous studies that the striatum contains high levels of D2. However, there was no relationship between extent of morphine CPP and D2 levels as revealed by [3H]-RAC binding. This finding is not consistent with the hypothesis that low levels of D2 receptors predispose a mouse to easy morphine conditioning. Further experiments are required to determine the ability to generalize our findings to other species and other drugs of abuse.

Using [3H] Spiperone to Detect Dopamine D2 Receptors in SD Rat Striatum Using the b-Imager. JOHN PIYIS (Nassau Community College, Garden City, NY 11710) THANOS PANAYOTIS (Brookhaven National Laboratory, Upton, NY 11973).

The dopamine D2 receptor is the main target of all neuroleptic drugs, and is therefore also one of the main targets of our studies. The density of this receptor is highest in the caudate and putamen, but is also found in low amounts in the temporal cortex, some thalamic nuclei, the pallidum, and some other brain regions. In spite of the low densities of DRD2 it has been suggested that the therapeutic efficacy of the neuroleptics is due to the blockade in these extra striatal regions, whereas the effects on motor activity are induced by receptor blockade in the striatum. Using [³H] Spiperone as a D2-dopamine receptor radioligand we can see the distribution of striatal DRD2 with the b-Imager.

Characterization of Foam Denuders for Sampling Pollutant Gases. KEVIN BRANDT (Lane Community College, Eugene, OR 97405) LAUREL EGENBERGER (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

This project investigated the collection efficiency and capacity of foam for removing gaseous pollutants from an air stream. Preliminary results indicate that an 80 ppi foam denuder can achieve 100% collection efficiency for SO₂ at a flow rate of 5 L/min. The size and mass of three foam disks are only about 2% of the annular denuder's, making the foam denuder smaller, lighter, cheaper and just as effective. A suitable foam denuder geometry for future development of a 5 L/min multi-pollutant sampler consists of 80 ppi foam, diameter 1.88 cm, total thickness 1.42 cm, and it can attain 100 % (no breakthrough) SO₂ collection efficiency.

The In Vitro Metabolism of Propyl Acetate in Blood and S-9 fractions of Male Sprague Dawley Rats. ALLISON CARTMELL (Gonzaga University, Spokane, WA 99352) TORKA POET (Pacific Northwest National Laboratory, Richland, WA 99352).

Propyl acetate (1-propyl acetate, CAS 109-60-4) is a solvent that can cause headaches, dizziness, drowsiness, and coughing at high vapour concentrations. To avoid typical solvent exposure symptoms, the current conservative exposure limit of 200 ppm has been established. However, little is known about the pharmacokinetics of propyl acetate. The purpose of this study was to determine the metabolic rate constants (K_M and V_{max}) for the metabolism of propyl acetate to its major metabolites, propanol (1-propanol, CAS 71-23-8) and propionic acid (CAS 79-09-4) respectively, in blood and S-9 fractions prepared from male Sprague-Dawley rats. Michaelis-Menten metabolic rate constants were obtained by quantifying the amount of the major metabolites produced from an initial propyl acetate concentration of 60 μ M or 600 μ M after an incubation time period of up to 20 minutes. The different Michaelis-Menten constant (K_M) for blood and S-9 fractions suggest that a different esterase is involved in the metabolism of propyl acetate to propanol in the blood and S-9 fractions. Although these esterases produce the same metabolites, the metabolic rate (V_{max}) is also very different. In S-9 fractions, propyl acetate is metabolized at 59.48 ± 8.246 nmol/min/mg to propanol, which is three times higher than the V_{max} in blood. The V_{max} for the metabolism of propanol to propionic acid is substantially lower than the V_{max} for the previous metabolic step. Propanol is much more slowly metabolized to propionic acid than the metabolism of propyl acetate to propanol. The blood and S-9 fractions having equivalent K_M metabolic rate constants, 17.98 ± 0.7384 μ M, for propanol to propionic acid metabolism suggest that the same esterase in blood and S-9 fractions is responsible for this second metabolic step. These metabolic rate constants will be applied to develop a physiologically based pharmacokinetic (PBPK) model in an attempt to assess the human health risks pertaining to propyl acetate.

NUCLEAR SCIENCE

Advance Fuel Cell Initiative Thermal Modeling. JEFFREY DAHL (Oregon State University, Corvallis, OR 97330) DANIEL WACHS (Argonne National Laboratory, Argonne, IL 60439).

Fuel temperatures are determined from axisymmetric thermal models for the Advanced Fuel Cell Initiative metallic and nitride fuels. Post Irradiation Examination also requires thermal fuel model analysis to determine temperature dependent element distribution caused by fission fragment migration. Fuel restructuring also in terms of void formation may also utilize results of thermal fuel modeling. The Systems Improved Numerical Differencing Analyzer/Gaski (SINDA/G) computer thermal modeling program is utilized to obtain temperature profiles for various cases which determine nominal and maximum heat load scenarios in the Advanced Fuel Cell Initiative (AFC-I) project. Axial and

radial thermal resistance of the fuel, sodium bond, cladding, helium gap, capsule and convection to coolant are accounted for in the fuel models. Safety analysis of fuel rod insertion into the Advanced Test Reactor is based on cladding and capsule temperature limitations. Modeling the distributed heat generation loads for normal operation loads of 33 kW/m and 39.6 kW/m for the off-normal limit, the determination of cladding failure is possible through analysis of temperature results. By utilizing the created fuel models in conjunction with the calculated heat distribution functions, temperature profiles may be obtained for a variety of developmental fuels.

Declad and Oxidize (DEOX) Head-End Reprocessing. *MICHAEL STAWICKI (Massachusetts Institute of Technology, Cambridge, MA 02139) KENNETH J BATEMAN (Argonne National Laboratory, Argonne, IL 60439).*

Several methods are currently being developed to reprocess spent oxide nuclear fuels. Two of these are the Uranium Extraction project at the Idaho National Engineering and Environmental Laboratory and the Pyrochemical Oxidation Fuel Project at Argonne National Laboratory West. These dissolution methods will be able to decrease fuel reprocessing time if they first employ a fuel decladding and pulverization process. The Declad and Oxidize (DEOX) process being developed at ANL-W is designed to meet these decladding and pulverization needs. The DEOX project's primary objective is to produce a product that can be used as high efficiency feed material for these two dissolution processes and then to gather as much data as possible about the behavior of spent fuel during DEOX processing. Specifically, DEOX is intended to remove greater than 95% of spent fuel from its cladding, while at the same time avoiding pulverization of the cladding that would contaminate the product. Its goal is to obtain a product particle size distribution with 90% by weight in a 45 μ m to 4mm band. Data will be collected on the extent of fuel oxidation as well as potential off-gassing of volatile fission products. DEOX is still in the developmental design phase. While experimental plans are being finalized, all necessary equipment has been designed and is being fabricated and tested. Initial findings indicate the equipment will meet all design criteria and should be ready for implementation by early September 2003 with first DEOX results available by the end of the month.

Occupational Safety for the Lead-Cooled Fast Reactor. *DAVID CULLEN (Brigham Young University, Rexburg, ID 83440) TODD ALLEN (Argonne National Laboratory, Argonne, IL 60439).*

This paper addresses occupational safety issues of the Generation IV lead-cooled fast reactor. The inherent safety features of a liquid-lead coolant have already been recognized. However, because of the nature of the coolant, there exists potential health and ecological hazards. The purpose of this paper is to show that with proper awareness, preparation and attention, working with the liquid lead-coolant can be a safe and reliable practice. The paper emphasizes the effects of inorganic lead on the adult human and outlines the governmental regulations concerning lead exposure. Further, the paper identifies situations in which operators of the lead-cooled fast reactor could come in contact with the lead-coolant, the forms of lead they may encounter in each situation, and the precautions and equipment that will ensure the operators' health and safety. As background, key physical and chemical properties, such as thermal conductivity and certain neutronics values, of lead as a coolant are compared and contrasted with those of other current and potential reactor coolants. The paper recognizes that the induced radioactivity of the lead-coolant poses the greatest human and ecological threat, and documents the production, concentration, and activity of various radio-nuclides that could be activated, giving emphasis to polonium 210. This leads to a discussion of lead-coolant disposal issues and options, including the methodology for classification of low-level radioactive waste. An outline of suggestions for future research on occupation safety for the lead-cooled fast reactor is also included. Such future research will continue to establish the safety case for the lead-cooled fast reactor.

Criticality of Plutonium/Uranyl Nitrate Solution with Gadolinium Neutron Poison. *WADE BUTAUD (Texas A&M University, College Station, TX 77840) J. BLAIR BRIGGS (Idaho National Engineering & Environmental Laboratory, Idaho Falls, ID 83415).*

The amount of fissile material that may be stored in one location is a concern that must be addressed by criticality safety experts who are responsible for the safety of nuclear operations. Many experiments were conducted in the mid 1900s involving criticality of a variety of fissile materials in a variety of different geometrical configurations. The measurement of critical solution heights were determined by E. D. Clayton and R. C. Lloyd for a plutonium-uranyl nitrate solution with varying amounts of gadolinium poison in a water reflected cylindrical vessel. In order to use these experiments, which were performed in the 1970's, as

a benchmark for modern-day applications a more detailed evaluation of these experiments is required. By identifying and analyzing uncertainties in these experiments, the overall uncertainty in the neutron multiplication, k_{eff} , was found using Monte Carlo methods such as those implemented in KENO 5.a and MCNP. From these calculations, benchmark models were derived. The evaluation of these experiments, including benchmark models and their associated uncertainties, will be published in an OECD NEA publication entitled, 'International Handbook of Evaluated Criticality Safety Benchmark Experiments' and will be available internationally to those who are seeking criticality safety information.

Information Download: Data Management Monitoring and Computing Analysis for STAR at PDSF. *ARIEL FLEMING (Tennessee State University, Nashville, TN 37209) DOUG OLSON AND ERIC HJORT (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

Data management and computing analysis for the Solenoidal Tracker at RHIC (STAR) is an essential effort to ensure efficient use of the limited computing resources. Trying to keep account of the usage of the Parallel Distributed Systems Facility (PDSF) computing facility and the number of files kept at the two different facilities, RHIC Computing Facility (RCF) and PDSF, becomes a very intensive job. Therefore the purpose of this research is to find a way to monitor the usage of the PDSF cluster and to keep account of the number of files each facility carries so that the datasets are the same. In analyzing the workload characteristics on PDSF (length of the batch jobs) over 3 years it was apparent that the most jobs were fairly long in the early years. As time progressed the jobs were shorter due to the fact that much of the activity was due to the analysis of the data. The software developed to count the files at RCF and PDSF has been an asset to researchers because now they have access to identifying the files that are needed at the facilities. This development prints the file monitoring results automatically to a web page making it easy to monitor the replication of files from RCF and PDSF. The research was very successful and useful because now researchers will be able to see how often the facilities are being used and they can tell the distribution of individual group usage to the facility.

Neutron Activation Analysis. *MARISOL CISNEROS (California State University Fresno, Fresno, CA 93704) ERIC B NORMAN (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

Neutron Activation Analysis helps scientists determine the identity of elements in unknown samples. Neutron Activation Analysis is the process of taking stable isotopes and adding a neutron to make them radioactive. By making the sample radioactive, a scientist can determine the identity of the isotopes by measuring the energies and half-lives of the gamma rays produced from the decays. The sample irradiated in this experiment was a standard pottery sample donated by Dr. Frank Asaro. The sample was sent to the McClellan Air Force Base, where the nuclear reactor is located, to be radiated one week before the sample was analyzed. On June 24, 2003, we visited the base to analyze the irradiated samples. This sample allowed us to see that isotopes with long half-lives. A second sample was irradiated the day of the trip so the short half-lives could be measured. After analyzing the sample, we figured out that there were approximately 30 elements in the sample. We were told that there were indeed 30 isotopes in the sample. However, upon further analysis of the data obtained at the reactor, we found that there were more elements in the sample that were not indicated, by Dr. Asaro, in the paper he published when he analyzed the sample himself. He said that indeed, there was more elements in that sample that were not reported in the original paper because they could not be verified using other methods.

Search for the Radioactive Decay of an Excited State of ^{18}Ne by Simultaneous Two-Proton Emission. *HAZIN WIN (University of Illinois at Chicago, Chicago, IL 60690) JOSEPH CERNY (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

For almost half a century, nuclear scientists have been searching for a radioactive decay mode involving simultaneous two-proton emission. Radioactive decay by sequential two-proton emission has been found and the search for simultaneous two-proton emission has continued. Although decay of radioactive nuclides is one possibility for two-proton decay, excited states of nuclei can also decay via this means. One such possible simultaneous two-proton emitter is the 1- state at 6.15 MeV in ^{18}Ne . At Lawrence Berkeley National Laboratory (LBNL), researchers are investigating the decay of ^{18}Ne using a radioactive beam of ^{14}O with an initial energy of 85 MeV. They are looking at the $^{14}\text{O} + ^4\text{He}$ reaction at 4.67 MeV with the help of the BEARS (Berkeley Experiments with Accelerated Radioactive Species) facility to produce ^{14}O . A special double sided silicon strip detector (S_{d}) with 48 concentric rings on the front surface and 16 radial sectors on the back surface will be used to detect the energies and the angular separation of two coincident protons. As a calibration for this detector, proton-proton collisions will

be used and therefore an understanding of these collisions is essential. It is also important to find a suitable AI degrader set that slows the 85 MeV ^{14}O beam down to about 4.7 MeV, where the ^{18}Ne , 6.15 MeV, 1- state formation cross-section has its maximum. In the first test run, the energies were measured after degrading an 88 MeV ^{16}O beam which is the analog beam of 85 MeV ^{14}O . This test-run showed that the technique works relatively well; the FWHM (Full Width Half Maximum) of the 5 MeV ^{16}O beam was only about 1.7 MeV. The main ^{14}O run will be in the fall.

Parametric Studies for U-233 Gamma Spectrometry. *CANDICE SCHEFFING (New Mexico Institute of Mining and Technology, Socorro, NM 87801) ALAN KRICHINSKY (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

Quantification of special nuclear material is a necessary aspect to assuring material accountability and is often accomplished using non-destructive gamma spectrometry. For U-233, gamma photons are affected by matrix and packaging attenuation and by a strong Compton continuum from decay daughters of U-232 (inherently found in U-233) that obscure U-233 gamma peaks. This project, based on current work being done at ORNL, explores the effects of various parameters on the quantification of U-233 at Building 3019A – including material form and geometry. Data collected for a period of three years from approximately 70 cans of stored U-233 was analyzed to identify factors influencing quantification. This previously established quantification method uses a series of gamma peaks emitted from U-232 progeny (at secular equilibrium) to identify a function that inherently adjusts for attenuation. The energy-dependent correction function for U-232 is applied to U-233 gamma peaks and allows for the content of U-233 in a container to be determined. A bias of almost 75% less than the actual U-233 mass was identified using this attenuation correction method. Controlled experiments using Zero-Power Reactor (ZPR) packets containing U-233 are now being conducted to determine the source of the bias and the influence of material geometry. These experiments control material distance, quantity and depth to examine the gamma-ray behavior to packaging, shielding, and self-attenuation. Results of these experiments demonstrated a slightly lower bias at approximately 57% less than the mass in the ZPR packets. There was also a direct correlation between the amount of attenuation occurring and the “goodness” of fit (R^2) for the initial attenuation function calculated using the U-232 progeny peaks. The R^2 value for any single scan did not have an effect on the overall bias of the experiment. The results showed that this attenuation function is not yet useful for quantifying U-233 at Building 3019A. More experiments are required to understand the relationship between the R^2 values and the attenuation. The source of the bias also needs to be understood at a more fundamental level for use of this quantification method.

Preliminary Baseline Cost Analysis Implementing UO₂-Steel Cermet SNF Multipurpose Casks. *JOHN NEERMAN (Roane State Community College, Harriman, TN 37748) JUAN J. FERRADA (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

With a growing inventory worldwide of depleted uranium (DU) in excess of more than 1.1 million tons, about half of which is stored in the U.S., the concern is rising surrounding the disposal of DU. Spent Nuclear Fuels (SNF) are also growing necessitating a systematically condensed disposal of both. The technology has been and is being developed to implement DU in the safe disposal of SNF via the addition of DU, in the form of uranium dioxide (UO_2), as a primary material with the design of SNF storage casks. Integrating the patent-pending invention by Dr.'s Charles Forsberg and Vinod Sikka, utilizing DUO_2 -steel cermet into SNF storage cask production, a preliminary baseline cost analysis has been performed to determine its feasibility and implementation. The analysis includes equipment design calculations, operation sequences and labor needs, site development and engineering, start up cost, and building design cost calculations to assess the capital investment and operation costs of this plant. Further information is still needed to finalize the analysis and posit a decision concerning continued development.

Research on Analysis of Integral Pressurizer Design in support of Nuclear Energy Research Initiative (NERI) Project. *GREG HEIHN (Texas A&M University-Kingsville, Kingsville, TX 78363) GRAYDON YODER (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

The International Reactor Innovative and Secure (IRIS) reactor is a new, pressurized water-cooled nuclear power reactor design. The reactor coolant system design incorporates a pressurizer, steam generators and eight reactor coolant pumps, all contained inside the reactor pressure vessel. The coolant system and its pressurization system are the main components used to improve efficiency and safety over existing reactor designs. Two potential Integrated Primary System Reactor (IPSR) pressurizer designs are being analyzed for this research project:

a steam pressurizer, and a nitrogen gas pressurizer. These two integral pressurizer designs differ from most conventional types because they incorporate a much larger interface more closely coupled to the reactor primary system. In the steam pressurizer design, the large interface between the saturated pressurizer and the subcooled primary coolant may lead to significant heat losses from the pressurizer and require a larger heater power to compensate. In the nitrogen gas pressurizer system, nitrogen diffusion from the pressurizer into the primary coolant can lead to significant quantities of dissolved nitrogen. Some postulated accidents have the potential to release this nitrogen as gaseous bubbles that could negatively impact heat transfer in the core. Engineering calculations examining heat transfer, mass transfer, and diffusion coefficients are being evaluated in order to determine the operational specifications to avoid these negative impacts. In addition to analytical calculations, a computational fluid dynamics model (CFD) of certain parts of the reactor, using the FLUENT code, will be created to determine the operational characteristics of the reactor. These calculations will combine thermal fluid and mass transport to produce an accurate simulation of the reactor system. The ongoing research in this project will combine the analytical calculations and CFD modeling techniques, implemented by the FaST team, to help understand details of the pressurizer operation.

Solutions of the OECD/NEA 3D MOX Benchmark Using the DOORS Code TORT. *JESSE KLINGENSMITH (Pennsylvania State University, University Park, PA 16802) JESS C. GEHIN (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

The purpose of this research is to extend the OECD/NEA 3D MOX benchmark, C5G7MOX, to test the three dimensional capabilities of TORT (Three Dimensional Oak Ridge Discrete Ordinates Neutron/Photon Transport Code). A similar problem was investigated in two dimensions and then modified to test the capabilities of modern three dimensional transport codes. Again, the reference solutions were found using MCNP (Monte Carlo N- Particle) and provided for comparison. The DOORS (Discrete Ordinates Oak Ridge System) code TORT was used to simulate four 17 x 17 fuel assemblies containing either UO_2 or MOX and to calculate the eigenvalue (effective multiplication factor) and relative fission rates for individual pins. Within the benchmark three different configurations corresponding to three levels of control rod insertion were explored. In general, TORT provides acceptable (less than 0.2% error) eigenvalues for little or no control rod insertion and less acceptable (0.5% error) eigenvalues for increased control rod insertion. The pin power accuracy is similarly affected by control rod insertion. The effect of increasing mesh refinement proved to be negligible for cases other than the coarsest meshes. The eigenvalues show an asymptotic behavior with increasing mesh refinement, which allows the user to employ a more coarse mesh refinement and be confident of the accuracy of the answer. The effect of increasing angular quadrature was found to change the bias-type error of the results. The initial increase in quadrature actually produces less accurate results, but there is evidence that the trend is reversed at even higher quadrature values and the results become more accurate. The errors associated with increased control rod insertion are mostly explained by the difficulty of modeling adjacent materials with very different cross section values. Increasing mesh refinement gave similar results to the two dimensional case, which is to be expected. The non-linear behavior of the eigenvalue results for increasing angular quadrature is not easily explained. Part of the behavior is probably due to variations in error cancellations, but further experimentation is needed to properly characterize and explain the results. The continuation of this project will be to explore further the effect of increased angular quadrature and to characterize the results as the simulation more closely models the actual physics.

LabVIEW DAQ for NE213 Neutron Detector. *MOHAMMED AL-AD-EEB (University of California, Berkeley, Berkeley, CA 94720) SAYED ROKNI (Stanford Linear Accelerator Center, Stanford, CA 94025).*

A neutron spectroscopy system, based on a NE213 liquid scintillation detector, to be placed at the Stanford Linear Accelerator Center to measure neutron spectra from a few MeV up to 800 MeV, beyond shielding. The NE213 scintillator, coupled with a Photomultiplier Tube (PMT), detects and converts radiation into current for signal processing. Signals are processed through Nuclear Instrument Modules (NIM) and Computer Automated Measurement and Control (CAMAC) modules. CAMAC is a computer automated data acquisition and handling system. Pulses are properly prepared and fed into an analog to digital converter (ADC), a standard CAMAC module. The ADC classifies the incoming analog pulses into 1 of 2048 digital channels. Data acquisition (DAQ) software based on LabVIEW, version 7.0, acquires and organizes data from the CAMAC ADC. The DAQ system presents a spectrum showing a relationship between pulse events and respective charge (digital

channel number). Various photon sources, such as Co-60, Y-88, and AmBe-241, are used to calibrate the NE213 detector. For each source, a Compton edge and reference energy [units of MeVee¹] is obtained. A complete calibration curve results (at a given applied voltage to the PMT and pre-amplification gain) when the Compton edge and reference energy for each source is plotted. This project is focused to development of a DAQ system and control setup to collect and process information from a NE213 liquid scintillation detector. A manual is created to document the process of the development and interpretation of the LabVIEW-based DAQ system. Future high-energy neutron measurements can be referenced and normalized according to this calibration curve. 1- MeVee: Unit used to equivocate electron absorption energy to other absorbed particles.

LabVIEW Data Acquisition for NE213 Neutron Detector. DHEVAN GANGADHARAN (University of California, Davis, Davis, CA 95616) SAYED ROKNI (Stanford Linear Accelerator Center, Stanford, CA 94025).

A neutron spectroscopy system based on a NE213 liquid scintillation detector at the Stanford Linear Accelerator Center measures neutron energies from a few MeV up to 800 MeV. The neutrons are produced from the electron beam and target interactions. The NE 213 scintillator, coupled with a Photomultiplier Tube (PMT), detects and converts radiation into electric pulses for signal processing. Signals are processed through Nuclear Instrument Modules (NIM) and Computer Automated Measurement and Control (CAMAC) modules. The processed pulses are then fed into a CAMAC analog to digital converter module (ADC). The ADC classifies the incoming analog pulses into one of 2048 digital channels. Data acquisition (DAQ) software based on LabVIEW version 7.0 acquires and organizes data from the CAMAC ADC. The DAQ system presents a spectrum showing a relationship between pulse events and respective charge (digital channel number). Various photon sources, such as Co-60, Y-88, and AmBe-241, are used to calibrate the NE213 detector. For each source, a Compton edge and reference energy in MeVee [1] is obtained, resulting in a calibration curve. This project is focused on the development of a DAQ system and control setup to collect and process information from a NE213 liquid scintillation detector. A manual is also created to document the process of the development and interpretation of the LabVIEW-based DAQ system.

PHYSICS

2Q-Low Electron Beam Transport Design for the Rave Isotope Accelerator Linac. ARTHUR REYNOLDS, JR. (Norfolk State University, Norfolk, VA 23504) RICHARD PARDO (Argonne National Laboratory, Argonne, IL 60439).

As proposed, the Rare Isotope Accelerator (RIA) Facility is a \$800 million plus, state-of-the-art continuous wave (CW), heavy ion particle accelerator for producing radioactive beams with primary beams of up to 400 kW of beam power. It is unique because it embraces the novel idea of simultaneously accelerating particles of two different charge states, the key reason for its ability to produce beams at such high intensities. Currently, scientists at Argonne National Laboratories, one of the two proposed sites for the new linac, are in the research and engineering design stages for RIA. They expect to have a complete baseline design by the conclusion of 2003. This paper describes the physical design for the first step of controlling and accelerating a two-charge-state beam. A low-energy beam transport system for two charge states (2Q-LEBT) has been modeled with beam optics codes. Diagnostics have been specified and the vacuum pumping system modeled. The results of these studies have been used to establish the physical beamline configuration and specify the necessary hardware for the 2Q-LEBT transport. The design will be used to build a 2Q-LEBT prototype on a selected site to serve as a test assembly for perfecting the generation, selection, and delivery of a one or two charge-state ion beam of adequate beam intensity to the remaining RIA driver linac.

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, 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, a more general resonance theory was developed that suggests the secondary electron energy distribution plays an important role in the resonant interactions. To determine the 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 this general resonance condition can better explain the measured electron cloud data in the storage ring at the APS for a variety of beam parameters.

Design and Construction of a Motorized Germanium Crystal Xray Beam Cleaner. LEONARD ERICKSON (University of Illinois, Urbana-Champaign, IL 61801) CARLO SEGRE (Argonne National Laboratory, Argonne, IL 60439).

Two devices are required for the process of choosing an energy from synchrotron produced x-rays: a monochromator for the filtering out the majority of the energies and a beam cleaner for removing the harmonics of the desired energy. MRCAT possesses both apparatuses, although the beam cleaner used is extremely high maintenance and a hassle to both set up and use. Designed around the bent germanium crystals already used in the current beam cleaner, the new beam cleaner promises to streamline installation and repeatability of alignment. As one of the goals of the new design was to keep the cost as low as possible, mill rotary stages, stepping motors, and several custom milled parts were used. When completed, MRCAT's new beam cleaner promises to decrease the valuable set up time for new users thereby increasing the time available for data collection.

Improved Rosenbluth Extraction of the Form Factors of the Proton: Analysis of Coincidence Data and Spectrometer Offsets. RYAN BEAMS (Wheaton College, Wheaton, IL 60187) JOHN ARRINGTON (Argonne National Laboratory, Argonne, IL 60439).

The extraction of the proton form factors G_E and G_M from electron-proton scattering using an improved Rosenbluth separation technique (measuring scattered protons) was conducted at Jefferson Laboratory by the Medium Energy group from Argonne National Laboratory. Consistency checks involving the background, cross sections, and dummy subtraction were conducted using coincidence data. The pion background was eliminated by imposing cuts using aerogels and gas cerenkov. The proton's differential cross section was extracted from the elastic peak and transformed using a Jacobian into an electron differential cross section for comparison. The thickness dummy end caps differs from the thickness of the target end caps. Overlaying the reconstructed γ -target spectrum without dummy subtraction with the dummy spectrum and integrating the end cap peaks provides a check of the dummy end cap factor. The coincidence data gave results different from the measure thickness, but in good agreement with other calculations. Accurately knowing the spectrometer angle and offset from the nominal target position are critical as the angle determines the kinematic. Using surveys, computer readings (LVDT), carbon pointing methods, and floor marks these uncertainties were appropriately addressed. The right arm spectrometer showed good agreement between the carbon pointing, the survey, and the LVDT. The left arm requires additional calibrations.

Laser Trapping of Radium Atoms in Order to Test Time-Reversal Asymmetry. AARON JACKSON (Morehouse College, Atlanta, GA 30314) ELAINE SCHULTE (Argonne National Laboratory, Argonne, IL 60439).

Laser trapping and cooling of atoms is a steadily growing field since initially introduced into the world of physics in the 1970s. Ever since its induction, a variety of avenues in the realm of high and medium energy physics have been opened to explore. Among the advances made possible by laser trapping/cooling include atomic interferometry, atom lithography, highly accurate atomic clocks, and parity non-conformation in electronic transition atoms to name a few. We are interested in the ability to use laser trapping in order to detect the electron dipole moment of Ra-225. The electric dipole moment, in conjunction with the neutron spin, electron momentum, and proton momentum, will be used to test the popular theory of time-reversal asymmetry. However, before the experiment can be performed on Ra-225, we use Ca metal and CaNO_3 to test the reliability of the laser trapping process. The two aforementioned samples are of particular desirability because calcium fluoresces with 423 nm photons that are readily available from an exist-

ing apparatus in the laboratory. Atoms can usually be treated as very small classical particles. However, the refractive index and absorptivity of atoms are strongly dependent on the frequency of the incident light. Therefore, the behavior of the atom at any time is dependent on the velocity of the atom (because of Doppler shifts). The frequency spectrum of the trapping beam is also important. Generally, atom trapping requires a laser beam tuned close to a transition frequency (spectral line) of the specific atom. Atoms will experience either attractive or repulsive gradient forces, depending on the detuning between the laser and the atomic transition. Future work in this area will include laser trapping of Ra-225 atoms in order to determine the validity of CPT symmetry and its impact on establishing conserved quantities in the laws of physics.

Measuring the Charge Radii of ^6He and ^3He . ANDREW GIAGNA-COVA (Lincoln University, Lincoln University, PA 19352) ZHENG-TIAN LU (Argonne National Laboratory, Argonne, IL 60439).

In this experiment we will be investigating the charge radii of ^6He ($\tau = 807\text{ms}$). We will be using the atom trap trace analysis (ATTA) method to trap the atoms. We are using ATTA because of its high trapping rate exhibited in the trapping of ^{81}Kr . This project has three phases, the first being ^6He production, the second is trapping the atoms, and finally measuring the charge radii. We will utilize the ion beam of the Argonne Tandem Linear Accelerator System (ATLAS) on a stationary target to produce the isotopes; the reaction of $^{12}\text{C}(^7\text{Li}, ^6\text{He})^{13}\text{N}$ has already been tested. This set-up will provide the isotope production to $10^7/\text{s}$. Due to its short $t_{1/2}$, the atoms must be pumped from the production chamber to the trapping mechanism quickly. To do this a turbo pump will be used. Atom trap trace analysis (ATTA) is a new method of ultra sensitive trace-isotope analysis. ATTA is based on the manipulation of neutral atoms. It is superior to other forms of isotope analysis in that it is not susceptible to contamination from other isotope other elements. The basis of ATTA is a modified magneto optical trapping system. The atoms in the system are slowed via a Zeeman slower while being cooled by a transverse laser, traveling in the opposing direction. ^6He will be in the $2^3\text{S}_1 - 2^3\text{P}_2$ transition to be trapped. Once trapped the atoms will be excited to the $2^3\text{S}_1 - 3^3\text{P}_2$ transition at 389nm. The atoms will be cooled, thus all Doppler line width will be well below the natural line width. The isotopic transition between these states will be measured and compared to the charge radii of ^3He . The charge radii of ^3He has been determined to be 1.9506 fm. By extrapolating this data the charge radii should be calculated.

Modeling Radiation Transport Using MCNP. BRIAN KREJCA (University of Massachusetts Lowell, Lowell, MA 01854) E. FRANK MOORE (Argonne National Laboratory, Argonne, IL 60439).

Designing nuclear instrumentation can be a costly process. Comparing various instrument designs helps reduce this cost. The probability that a detector detects radiation, also known as efficiency, is among the most important criteria considered when evaluating new designs. Computer modeling of radiation transport through a detector would allow designers to estimate the efficiency of their design. Currently, the most common design of a gamma ray detector consists of a cylinder of high purity Germanium, a semiconductor crystal, since it produces the best energy resolution. However, the size of the crystal is limited by manufacturing technology, so the overall efficiency of a single detector is relatively low. The Gammasphere array employs more than 100 detectors of this style. Even though Gammasphere is currently the best instrument for gamma ray spectroscopy, at an approximate cost of \$25M, there is room for improvement. Also, Gammasphere may not have the optimum geometry for all experiments. For these reasons, designs for the next generation of gamma ray spectroscopy instruments have been worked on for many years. Using the computer program known as the Monte Carlo N-Particle Transport Code (MCNP), the efficiency of a nuclear instrument design can be estimated. Several existing and emerging designs are evaluated here. Simulated results are then compared to experimental results for evaluation of the modeling method. With a valid modeling process, combinations of detectors can be evaluated to optimize their geometrical arrangements for overall efficiency, which is paramount when designing the next level of gamma ray spectroscopy instruments.

Optical Production of a Beam of Metastable Krypton. WILLIE WONG (Princeton University, Princeton, NJ 08544) LINDA YOUNG (Argonne National Laboratory, Argonne, IL 60439).

Metastable beams of noble gas atoms have a wide range of applications from industrial uses to basic research. The high internal energies of the metastable states make them suitable for lithography, while the laser manipulations afforded by the lowering of the transitional energies allow the study of basic properties such as isotope shifts or Bose-Einstein Condensates. One important application of metastable noble gas and the laser techniques thereof is the analysis of rare isotopes. The low level counting techniques in trace analysis could in principle allow

the dating of underground water or polar ice cores via the radioactive ^{81}Kr isotope. The current research, however, is limited by the efficiency of the metastable source. This paper demonstrates an optical method (compare to previous discharge methods) of producing a beam of metastable krypton, which, when compared to current state-of-the-art r.f. sources, shows a preliminary result with similar metastable flux density (3×10^{14} atoms $\text{s}^{-1} \text{sr}^{-1}$). With further optimizations, the method presented in this paper promises at least two orders of magnitude gain. However, due to the higher total flux density of our beam, it doesn't yet surpass the r.f. beam in terms of production efficiency, which hopefully can be solved with further optimizations. On the other hand, the method presented in this paper is easily generalizable to the production of metastable atomic beams of other noble gases such as argon or xenon.

Preparing Experimental Equipment for Testing Time-Reversal Asymmetry. SARAH HICKS (Florida State University, Tallahassee, FL 32306) ELAINE SCHULTE (Argonne National Laboratory, Argonne, IL 60439).

Time-reversal (T) invariance is one of the symmetries important in quantum field theory. The CPT theorem states that if charge conjugation (C) and parity (P) of a particle is violated, then T is violated as well. There have been direct observations of a CP violation through decays of K mesons; however a debate over observation of T violation alone continues. The overall goal of a new experimental program is to observe a T violation without invoking CPT theorem. A permanent electric dipole moment (EDM) is parity and time-reversal violating in nuclei and atoms. Under T-reversal, the spin is reversed, but the EDM remains constant. The sample that will be used will be 225-Radium due to its long lifetime and desirable spin of 1/2. Before the experiment begins, an oven must be constructed. Calcium will just be used instead of 225-Radium to test the oven. Both elements are alkaline earth metals; thus Ca may have similar chemical properties to 225-Radium. Samples of Ca will be placed inside the oven and detected by laser fluorescence.

Radio Frequency Quadru-pole Ion Guide Assembly: A Perspective on the Concerns and Requirements of Assembling an RFQ. SCOTT BATCHELOR (Morehouse College, Atlanta, GA 30314) GUY SAVARD (Argonne National Laboratory, Argonne, IL 60439).

Interest in the area of rare and short-lived isotopes is on the rise. In order to study these isotopes/ions successfully a new type of accelerator must first be developed to meet the specific criteria to make this once thought impossible task a reality. The proposed Linear Accelerator RIA or Rare Isotope Accelerator is the apparatus that will produce these short-lived isotopes in abundant quantities. Yet before RIA can be built, several technological advancements must first be made. One of these necessary advancements is a way to cool down or remove energy (several orders of magnitude) from the ions before they reach their final destination. A project currently running at Argonne is dedicated to producing a gas cooler that can perform this task. Since its construction, the experimental gas cooler has produced exceptional results that are promising as well as encouraging. Still it is the general consensus that better results and more specifically better efficiency can be achieved. Under the guidance of Guy Savard it has been my primary objective during this appointment to assemble and test different components that are required to enhance results on the RIA Gas Cooler. These components consist of a pair of Radio Frequency Quadru-poles (RFQ) and the necessary transformer circuits to control the RFQ's. The Radio Frequency Quadru-pole's have been designed to stabilize the ions of interest after they have exited the nozzle on the RIA Gas Cooler. The two RFQ's and the transformer control units will be placed in two separate sections under vacuum (Section 1 at 10^{-1} Torr and Section 2 at 10^{-3} Torr) after the Gas Cooler nozzle. Given the appropriate pressure, RF and DC potential, it is believed that the RFQ's will be able to stabilize and guide the now low energy ions to their final destination.

Radio Electric Dipole Moment Project. PATRICK SALCIDO (Richard J. Daley Community College, Chicago, IL 60652) ELAINE SCHULTE (Argonne National Laboratory, Argonne, IL 60439).

This is a project to build a prototype Electric Dipole Moment (EDM) detection region. The ultimate goal is to detect the EDM of Radium 225 (^{225}Ra) atoms. Many challenges exist detecting the electric dipole moment. Stray electric currents cause magnetic fields, altering the precession of the atom in question. High voltage must be used in conjunction with a weak magnetic field to detect the EDM. Background noise is a major problem with projects like these, because currents in the pico and nano amp range can cause spurious EDM signatures. Background noise, if not properly controlled, reaches and well exceeds these ranges. Electric field plates need to be conditioned with these high voltages to overcome leakage currents. Argon gas can be used to help "scrub" the plates and reduce leakage currents and have high volt-

age avalanche. Though the project is at its infancy, significant progress has been made to eliminate the problems with high voltage.

Semi-Automatic Steering Algorithm, Beam Control and Alternate Method of Determination of Emittance at the NICADD Photoinjector Laboratory. JASON WENNERBERG (*University of Illinois at Chicago, Chicago, IL 60607*) PHILIP PIOT (*Argonne National Laboratory, Argonne, IL 60439*).

The Northern Illinois Center for Accelerator and Detector Development (NICADD) has a facility at Fermi National Accelerator Laboratory (FNAL) called the Fermilab NICADD Photoinjector Laboratory (FNPL). On site, the machine is referred to as the A0 photo-injector or A0pi. This facility is an 18 MeV electron linear accelerator used to investigate accelerator technologies. This accelerator produces a high intensity, low emittance electron beam, used to study plasma wake-field acceleration, channeling radiation, and flat beam production. This paper summarizes the work I conducted at this facility designing a software package to consolidate the beam control systems, to semi-automate certain processes currently performed by hand and to allow for some methods of measurement not currently possible with distributed systems on different platforms.

Simulations of Beam Dynamics in the ATLAS Linear Accelerator as Part of a Post Accelerator for RIA. ALAN HOFFMAN (*University of Chicago, Chicago, IL 60630*) PETER OSTROUMOV (*Argonne National Laboratory, Argonne, IL 60439*).

The proposed Rare Isotope Accelerator (RIA) plans to incorporate sections of the existing Argonne Tandem Linear Accelerator System (ATLAS) as a post accelerator for radioactive beams. This proposal necessitates a better understanding of the dynamics of low-velocity, heavy-ion beams in ATLAS. Accurate simulations of beam runs are needed not only to understand the trajectory of accelerated charged particles, but also as an efficient method of tuning the resonant cavities. Using CST Microwave Studio we modeled the accelerating cavities in ATLAS and numerically calculated their internal electric and magnetic fields. We then used Trackv32 to simulate the dynamics of uranium +34 ion beams in each of the three linear accelerators that make up the ATLAS facility. Preliminary beam matching for the transitions between ATLAS sections was performed using Trace 3-D. The models are consistent with experimental conditions and simulations are progressing well. The size of the beam envelope in simulated runs is small compared to the aperture size of the resonant cavities. For future studies, our simulation method will be modified to include other proposed portions of the RIA post accelerator. In the proposed RIA facility, operators will use our simulation method in routine linac tuning, which should help prevent unnecessary down time and provide for more efficient research.

Two Improvements to the Canadian Penning Trap System. JEFFREY LETCHER (*Kalamazoo College, Kalamazoo, MI 49006*) GUY SAVARD (*Argonne National Laboratory, Argonne, IL 60439*).

The Canadian Penning Trap (CPT) is a high precision mass spectrometer operating on-line at the Argonne Tandem Linac System (ATLAS). As part of a project to modify and improve the CPT system, a quadrupole deflector was simulated and designed, and the efficiency of a Micro-channel Plate (MCP) system currently used was explored. The quadrupole is a necessary component for flexible alteration of the ion beam line for the future installment of the Advanced Penning Trap (APT). After modeling various quadrupoles, a circular plus shim electrode combination was settled upon. While the estimated voltages differ slightly from similar existing models, this design still functions successfully. The MCP currently has an absolute efficiency of about 50% and it was felt this could be improved. Through literary research it was determined that floating the voltage of the MCP system was the best way to significantly increase the efficiency of the detector. Experiments to verify this are currently underway. It was also determined that the addition of a grid in front of the MCP would most likely have little positive effect on the efficiency of the system.

Vacuum System Automation of the Canadian Penning Trap Injection System. DANIEL PENG (*Princeton University, Princeton, NJ 08540*) GUY SAVARD (*Argonne National Laboratory, Argonne, IL 60439*).

The Canadian Penning Trap (CPT) is a mass spectrometer designed to measure nuclide masses to high precision. Modern experiments in nuclear physics require the maintenance of high vacuum levels throughout the volume of the experiment for the unimpeded passage of particle beams, and the injection system of the Canadian Penning Trap (CPT) is no exception. Maintaining the injection system vacuum requires 8 mechanical roughing pumps, 9 turbomolecular pumps, and 20 valves, and monitoring it involves 18 thermocouple gauges, ion gauges, and convectron gauges. Moreover, the CPT injection system

presents a special challenge in fault protection, as its gas cell stops the reaction products in 150 torr of helium gas separated from vacuum by a thin metal window whose breaking point is little more than 150 torr . Keeping this thin metal sheet intact is of vital importance in the case of a pump failure, since its rupture could spread radioactivity throughout the interior of the Enge spectrograph, rendering it inoperable for a period of up to several months. Through robust software engineering and careful system design, the new Modicon 984 Programmable Logic Controller (PLC) for the CPT injector provides a safe and easy way to vent and pump down the system. It monitors the vacuum system for failure through a set of MKS 937, MKS 937A, MKS 286, and MKS 290 gauge controllers and a set of Leybold NT150/360, Leybold NT151/361, Leybold NT20, and Osaka TC-440 turbomolecular pump controllers. The PLC thus directly monitors gauges and controls the valves, roughing pumps, and turbomolecular pumps in the vacuum system, permitting it to resolve vacuum problems thousands of times faster than human intervention could. The PLC now forms a necessary part of the day-to-day operation of the CPT.

A Production Database for Cathode Strip Chambers of the ATLAS experiment. MARC MCGUIGAN (*College of William and Mary, Williamsburg, VA 23186*) KETevi ASSAMAGAN (*Brookhaven National Laboratory, Upton, NY 11973*).

Brookhaven National Laboratory (Upton, NY) is responsible for designing and constructing Cathode Strip Chambers (CSC) for the ATLAS detector. Before a chamber can be installed in ATLAS the tension in each wire must be tested to ensure that it will perform correctly. The goal of this project was to organize CSC tension data in a database format so that researchers can easily view and compare data. Prior to this project, the tension data had been stored in files with a .dat extension. The first task was to convert the existing files into a database. The programming software, LabVIEW 6.1 was used to transfer the existing files into one Microsoft Access 2000 database. After successfully transferring past files, the program that operated the tension tests was modified so that the data from future measurements will be written directly to a Microsoft Access 2000 database. The data for all future CSC tension tests will be written into the database that contains the existing tension data.

Calorimeter Calibration for Particle Detection. BLENDELL REGISTER-WHEATLE (*Broward Community College, Davie, FL 33314*) CAROL SCARLETT (*Brookhaven National Laboratory, Upton, NY 11973*). The Lifetime of a K_L^0 is approximately 10 nanoseconds (10ns). This particle can decay into several daughter particles. The branching ratio for a $K_L^0 \rightarrow \pi^+ \nu \bar{\nu}$ is 3×10^{-11} according to the standard model. This means that it is predicted that 3 out of a hundred billion K_L^0 decays will end up a $\pi^+ \nu \bar{\nu}$ particle. In order to prove or disprove this calculation, the energy left behind (in the form of a photon) from cosmic ray muons were used to calibrate calorimeters. The energy of the Photon and the direction it was traveling allow us to reconstruct the original particle. The calorimeters, which consisted of a photo multiplying tube (PMT) and scintillating material, will eventually be part of the detection system of the KOPIO experiment. After calibrations were all done, we found that there was a difference by as much as 37% between the calorimeters. Once the difference in the PMT gain has been accounted for, the difference in the mean of the calorimeter distribution must come from a difference in calorimeter efficiency.

Gluon Density in Heavy Ions. REBECCA LAMB (*Rensselaer Polytechnic Institute, Troy, NY 12180*) LESLIE C BLAND (*Brookhaven National Laboratory, Upton, NY 11973*).

Current theory suggests that the gluon density within hadrons reaches a saturation point at very small probing wavelengths. It is also theorized that gluon density is enhanced in heavy ions such that gluon saturation may be observed in the forward region at the collision energies of RHIC. Measurements taken with the Forward d^0 Detector (FPD) at STAR aim to probe relative gluon densities in deuteron and gold ions. This is observed via the high energy d^0 s produced from the scattering of an incident quark and a gluon. The FPD is a calorimeter that primarily detects high energy photons resulting from d^0 decays at large pseudorapidity. This analysis begins the process of extracting gluon density information about the gold nucleus. This is accomplished by observing d^0 s in the direction of the deuteron beam. d^0 s are detectable in the data set and significant progress has been made in gain matching the data. A preliminary energy scale has been determined, which produces an invariant mass peak with a sigma of $0.035 \text{ GeV}/c^2$. This energy scale is the critical quantity which allows comparison between proton-proton and deuteron-gold collisions. More analysis needs to be done before any conclusions about gluon density can be reached.

Mapping the Magnetic Field of the PHENIX Inner Coil. JOHN KE-HAYIAS (Columbia University, New York, NY 10027) ACHIM FRANZ (Brookhaven National Laboratory, Upton, NY 11973).

The Pioneering High Energy Nuclear Interaction Experiment (PHENIX) at the Relativistic Heavy Ion Collider (RHIC) added an Inner Coil to their Central Magnet about a year ago. This coil can greatly change the magnetic field in the region close to the beam pipe. The magnetic field will bend a charged particle's path, and this is used to calculate the momentum. For this reason, it is important to have a precise map of the magnetic field to use during event reconstruction. TOSCA simulations of the Inner Coil were run at Los Alamos National Laboratory. This data was plotted with the software library ROOT to show how the magnetic field and integrated field (IB·dl) changes with the Inner Coil in phase (higher momentum resolution) or out of phase (for a future silicon detector around the beam pipe) with the Outer Coil, and at varying strengths. The effect is seen within the first 80 cm in the r direction – out of phase the field can be decreased to 0 gauss at the center, in phase it can be increased to about 9000 gauss. The integrated field shows a similar effect – a value of 0 gauss-cm in the first 20 cm of r for the out of phase configuration, and a greatly increased overall value with the in phase configuration. The hardware from the 1998 mapping of the PHENIX magnets provided the Hall probes mounted on plates and ribbon cables for reading off the voltages. A Keithley 7002 switch and 2000 multimeter were used to test the cables. They both take GPIB commands, and a C++ program was written to control the data taking remotely, via a Tektronix AD007 GPIB to Ethernet adaptor, for the future mapping. The actual mapping will take place in the near future, although everything has been prepared.

Mixed Apparatus for Radio Investigation of Atmospheric Cosmic-rays of High Ionization (MARIACHI). KRISTA FEIERABEND (Long Island University, Southampton College, Southampton, NY 11786), TARA FALCONE (SUNY at Stony Brook, Stony Brook, NY 11974) HELIO TAKAI (Brookhaven National Laboratory, Upton, NY 11973).

These days, the study of physics in the energy scale of 106 TeV (1018 eV) and beyond is only available by means of studying ultra high energy (UHE) cosmic rays. In order to make use of these unusual events, large area detectors are required. Conventional detector technology can cover areas up to a few thousand square kilometers and is extremely costly. A more resourceful way of investigating UHE cosmic rays may be to use a technique known as radio meteor scatter (RMS). RMS is a process that has been used to study meteorites and micrometeorites, and involves applying continuous radio waves over a wide area. Therefore, if this technique can be used for the detection of UHE cosmic rays, we can cover a much larger area with a lesser amount of cost. However, the detection of events alone does not essentially provide information about the physics behind the phenomena. Consequently, in order to identify cosmic ray signals and extract shower parameters from them we are designing an experiment combining the radio scatter technique along conservative muon detectors put in coincidence. High school teachers involved in the BNL/SUNYSB QuarkNet outreach program are aiding in the setup of the muon detection systems which will be installed in physics classrooms of several local school districts on Long Island.

Study of Direct Photon Production from Polarized Proton Collisions Observed with the PHENIX Detector During Run II of RHIC.

ARTHUR LIPSTEIN (Columbia University, New York, NY 10027) GERRY BUNCE (Brookhaven National Laboratory, Upton, NY 11973). Deep inelastic scattering experiments over the past two decades have revealed that only about 30% of the proton's spin is carried by its quarks. Although the remaining 70% of the proton spin may reside in the spin of the gluons and/or the orbital angular momentum of all the partons, these contributions have yet to be measured precisely. Since the production of direct photons in proton-proton collisions is dominated by the quark-gluon interaction $q+g \rightarrow \text{gamma}+q$, direct photon production is a key probe for measuring the gluon distribution in the proton in the framework of perturbative QCD. As a result, the study of this reaction should allow for future investigations of the polarized gluon distribution if polarized proton beams are used with the appropriate combination of bunch spin helicities. In this paper, a method is investigated and a first attempt is made to identify direct photon production in proton collisions at $\sqrt{s}=200$ GeV using the data collected by the PHENIX collaboration in RHIC Run II. A direct photon signal was extracted by identifying direct photons on an event-by-event basis as well as by employing a statistical approach which looked at the difference between photon yields resulting from meson decays and the total inclusive photon yield produced by the proton-proton interaction. Data collected in the central rapidity region of the PHENIX electromagnetic calorimeter was primarily considered.

Visualization and Energy Measurement of Laser Pulses in the Presence of Noise. MICHAEL POLYAKOV (Carnegie Mellon University, Pittsburgh, PA 15213) KARL KUSCHE (Brookhaven National Laboratory, Upton, NY 11973).

Spiricon Pyrocam III is a high performance digital camera for infrared laser beam viewing. Its use in our lab will be to capture short laser pulses from the CO₂ laser system. In such a case external triggering or video trigger are required. I will discuss different modes of operation of the Spiricon Pyrocam III camera and the problems encountered while operating in those modes. Besides acquiring snapshots of laser beam with Spiricon's camera, Moletron detectors are used to measure the energy of the incoming pulse. There are a variety of detectors with different voltage responsivities and properties. However, a method to visualize the signals from a variety of those detectors is currently lacking. Also, a method has to be devised to reconstruct the amplitude of incoming signals from the surrounding noise. Here, such an algorithm is suggested, which is based on prior knowledge about the shape of the pulse. Simulation results and the algorithm application for Moletron detectors are discussed.

Possible Feed Down of Drift and Snapback Effect in Tevatron Dipole Magnets. RICHARD BERGGREEN (Pomona College, Claremont, CA 91711) PHILIP SCHLABACH (Fermi National Accelerator Laboratory, Batavia, IL 60510).

The Tevatron Superconducting Dipole Magnets have been functioning in the Main Ring at Fermi National Accelerator Laboratory for approximately 20 years. During this time, the Magnet Test Facility has been studying the characteristics of typical magnets from the ring. The most recent tests conducted were to determine if the relatively large lower-order multi-pole coefficients were due primarily to the geometry of the magnet or to the testing method. This was done to help determine if actions need to be taken within the Tevatron to correct the errors in the dipole field. The testing, done using a rotating coil probe system, returned data that served to split the original question into multiple parts. The first magnet, tb0269, demonstrated drift in its skew quadrupole (a1) that bore a striking resemblance to the drift demonstrated in the built-in normal sextupole. Other magnets also demonstrated drift, but without the similarity in shape. This leads to questions about whether this drift is in fact due to the feed-down of the built-in sextupole, as would be indicated by the similarities in shape, or due to another factor (e.g., coil geometry). Another indicator that was used to further lessen the likelihood of the feed-down is that with the correct geometric for the hysteretic, the width is incorrect, and vice versa. This indicates that the built-in sextupole is not feeding down because the feed-down would have similar geometry and hysteretic loop.

A Slice of Pi in the Sky: Star/Galaxy Catalog for the Nearby Supernova Factory. MARC RAFELSKI (University of Arizona, Tucson, AZ 85721) GREG ALDERING (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The Nearby Supernova Factory group focuses on observing many supernovae in order to better determine their characteristics. Supernovae are used to determine the expansion history of the universe. To find supernovae we have observed two pi steradians (solid angle) of the sky. To discover supernovae, new images are subtracted from reference images created at an earlier time. This process often also flags non-supernovae, such as misalignments, asteroids, and variable stars. In order to decrease the number of false supernova candidates, a catalog can be used to identify stars and variable stars. In this way all star candidates can be masked since they are not supernovae candidates. We present software that creates a catalog of the images with star and galaxy classifications. The software uses a neural network in the program SExtractor to do the object classification. The program stores the results in an SQL database in preparation for the master catalog. After all the data has been processed with this software, our catalog will reduce false supernova candidates caused by stars and variable stars. The catalog also yields much information on the image quality, which can be used in the creation of a master reference. Furthermore, it can be used for many other scientific pursuits, such as finding variable stars, gamma ray burst after glows, and other transient objects. Finally, when completed this catalog will be the largest CCD survey available.

Analytic Study of Envelope Modes for a Fully Depressed Beam in Solenoidal and Quadrupole Periodic Channels. BORIS BUKH (City College of San Francisco, San Francisco, CA 94121) STEVEN LUND (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

We present an analysis of envelope perturbations evolving in the limit of fully space-charge depressed (zero emittance) beam in periodic thin-lens focusing channels. Both periodic solenoidal and FODO quadrupole focusing channels are analyzed. The phase advance and growth rate of normal mode perturbations are analytically calculated as a function

of the undepressed particle advance to characterize the evolution of envelope perturbations.

Cooling the Catcher: Using a Liquid Nitrogen Cold Finger to Trap Atoms. CHRISTOPHER BORQUEZ (CSU Fresno, Fresno, CA 93726) ALI BELKACEM (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

Ali Belkacem and his research team at the Lawrence Berkeley National Laboratory have been studying the behavior of electron orbitals around atoms during ionization. The team analyzes these electron orbitals by ionizing atoms using X-rays, laser, electron beams, or a combination of each. With an electrical pulse, the ionized atoms are directed toward a Micro Channel Plate (MCP) that can detect flight times of the ions. When lasers are used for ionization, data becomes cluttered by signal from background gas. We designed a Liquid Nitrogen Dewar to cold finger assembly to freeze out, or 'catch' background gas. Most of the background gas is trapped when the atoms come in contact with the cold temperature of the catcher and freeze. A foam insulated dewar was used in early experiments to feed the cold finger, but held Liquid Nitrogen for only one half-hour. A vacuum insulated dewar would continually supply the cold finger with Liquid Nitrogen for hours because the vacuum eliminates convection and there are very few points of conduction on the dewar openings. A specialized vacuum insulated dewar was designed and multiple set-ups were tested. Results indicate that the new dewar can hold liquid nitrogen and efficiently cool the catcher for over four hours.

Creating The "Universe Adventure" Website. ARTIE KONRAD (UC Berkeley, Berkeley, CA 94720) MICHAEL BARNETT (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The Particle Data Group at Lawrence Berkeley National Laboratory is creating a website entitled, 'The Universe Adventure'. Recently, the group designed a poster that explained theories about the history and fate of the universe. The objective of the website is to 'flush out' the poster with more fact and theory about cosmology. Macromedia Flash, was the main application used for creating the website, but Adobe Photoshop and Illustrator were also vital applications. After a draft of each page was created (with particular attention to aesthetics and creativity), the content was reviewed by astrophysicists to ensure accuracy. Since the primary objective of the website was to answer questions from the poster, we organized the website into categories of these questions. Students can navigate easily to the pages that answer their specific questions. The pages focus entirely on cosmology and explain topics from the Big Bang to the expansion, size, and age of the universe. The website is fun, animated, colorful, and easy to navigate through. Overall, it does a good job of clearing up many questions, while taking the student on an exciting adventure through the universe.

Demonstration of the Meissner effect Using Superconducting Y₂BaCuO₇(YBCO). MICHAEL MOORE (College of the Redwoods, Eureka, CA 95501) STEPHEN GOURLAY (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The Superconducting magnet department at LBL needed a demonstration of the future uses and benefits of superconductivity other than magnet design. It was decided that a working model of a Superconducting levitation train would be an excellent example of diamagnetism, flux pinning and the Meissner effect. The train consisted of 3 hexagonal YBCO pieces nestled in a foam box which doubled as a reservoir for the liquid nitrogen needed to bring the YBCO below its critical temperature T_c of 80 K. For the track, NdFeB magnets were arranged 3 wide with a north-south-north configuration so that the YBCO was always in a field where the equipotential planes were parallel to the trains desired motion. The magnets were glued to Iron base pieces to achieve the desired racetrack shape, and then attached to a sufficiently large rectangle of plywood outfitted with handles for easy transport. For aesthetics, the outside of the foam box was covered with digital images of an LBL shuttle bus making the train a familiar site to everyone at the lab, and the plywood was covered with a sand flooring, trees and shrubs for the public demonstration. The project was a success after a few revisions of the train and track design. There is plenty of room for research into diamagnetism, flux pinning and the Meissner effect. While this is only a demonstration and promotional tool, it may also serve as a starting place for future study into these properties of high temperature superconductors.

Growth and Characterization of Co/Pt (100) Multi-layers. TANINA BRADLEY (North Carolina A & T State University, Greensboro, NC 27411) BYRON FREELON (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The continuing effort to increase computer storage capacity has led to an increased interest in epitaxial growth. Epitaxial grown multi-layers

have been used to increase storage capacity of hard drives, and now are being studied for possible improvements. Our goal is to determine if adjusting growth parameters will affect magnetic properties of Co/Pt (100) multi-layers. In particular, we are interested in increasing the structural domain sizes in Co/Pt multi-layers. The multi-layers are grown on a Si₃N₄ membrane using Molecular Beam Epitaxy (MBE). During growth, the surface structure is observed and characterized using Reflection High Energy Diffraction (RHEED). The magnetic domains are observed by using an X-Ray Magnetic Microscope, named XM-1, at the Advanced Light Source.

Natural Terrestrial Radioactivity. REYNA ALARCON (CSU, Fresno, Fresno, CA 93704) TOM KNIGHT (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

As part of the intensive research institute, our involvement in this workshop consisted of understanding natural terrestrial radioactivity; providing a perspective on the radioactive elements present, their intensities encountered at various locations, and its significance to human health. There are three categories to identify radioactivity found in nature; primordial (has been around since the creation of Earth), cosmogenic (was formed as a result of cosmic ray interactions), and human produced (either enhanced or formed due to human actions). Natural radiation is present in materials such as soil, rocks, floors, walls, gas, oil, food and water. Radioactive elements that decay quickly pose health risks to humans yet certain radioactive materials have been beneficial to medicine, industrial and environmental breakthroughs. Uranium 238 and Thorium 232 are elements with long half-lives found in the environment. Using soil samples and the germanium detector we were able to count the gamma ray peaks of decays of these elements. Applying quantitative analysis we were able to calculate the mass concentration of each radioactive element was present in our sample. The history of how radioactive elements have been used has also been important for homeland security due to the various possibilities of nuclear attacks. A possibility of providing homeland security checks has arisen with the concept of using auto engine air filters to collect radioactive element found in the area and detect any elements that should not be present.

Strong Gravitational Lensing Candidates in the Hubble Deep Field North GOODS Data. REBECCA NICODEMUS (Purdue University, West Lafayette, IN 47906) GEORGE SMOOT (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

In this study, we search the HDF-N GOODS ACS Version 0.5 survey for strong gravitational lenses. Strong gravitational lensing is explained by Einstein's General Theory of Relativity and allows us to address many fundamental questions in astrophysics. The data released in June 2003 includes Epochs 1-4 of the HDF-N with the VIZ bands in all Epochs and B band in Epoch 1. SExtractor was employed to make an initial catalog of objects in the survey that included galaxies, stars and cosmic rays. SExtractor detected 60795 objects covering approximately 161 square arcminutes. Hyperz was then employed to determine the photometric redshifts of the objects in the catalog. Hyperz was able to determine 17989 photometric redshifts. A program was written in MATLAB to find two objects within eight arcseconds and within 0.04 redshift of each other. A total of 1875 pairs were found in the survey. Further work includes employing the upcoming Version 1 release in search of doubly and quadruply imaged sources.

Third-Order Autocorrelator for Measuring Pulse Contrast in a Multi-Terawatt Laser System. LUKE WOLCOTT (Swarthmore College, Swarthmore, PA 19081) WIM LEEMANS (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

In the innovative acceleration schemes being explored by the L'OASIS group at the Lawrence Berkeley National Lab, high-intensity laser pulses travel through plasma, accelerating electrons in their wake. Due to the high intensity of these 50-femtosecond pulses, minute pulse shape characteristics can significantly alter the laser-plasma interaction. Third-order autocorrelation of a laser pulse, using the nonlinear processes of frequency doubling and sum-frequency generation, provides a powerful diagnostic tool capable of obtaining high dynamic ranges. We developed and optimized a third-order autocorrelator to look at the fundamental shape of the laser pulses generated in the L'OASIS lab at the Center for Beam Physics. This diagnostic will allow us to measure pulse contrast and shape of the 10- and 100- terawatt laser systems.

Vertical Beam-Position Stabilization on a Synchrotron-Light-Source Beamline. JOE SZURLEY (Lake Tahoe Community College, Lake Tahoe, CA 96150) FRED SCHLACHTER (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

X-ray interactions with matter serve as one of the most important tools in understanding atomic and molecular structure. A synchrotron light source produces bright beams of photons in the ultraviolet and X-ray

regions of the spectrum and is thus a valuable probe of the atomic structure of matter. A beamline and monochromator must deliver a monochromatic beam of photons with good positional stability to obtain high-quality data. A feedback system was installed at the Advanced Light Source on beamline 9.3.1 to reduce position instabilities in the beam and to allow reliable and repeatable measurements. The system provides beam stabilization by detecting fluctuations in the vertical beam position and by feeding back corrections to the piezo actuator controlling vertical beam position. Intensity and position of the beam were measured with feedback on and feedback off as energy was scanned to demonstrate proper functioning and improved performance of the beamline. Analysis of data obtained shows vertical beam position stability and intensity have both improved by a factor of 3. This helps further the capabilities and repeatability of data collection on the beamline.

Wavelet Analysis of Supernovae Spectra. VIDYA VASU-DEVAN (Columbia University, New York, NY 10027-8361) GREG ALDERING (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).

The Nearby Supernova Factory is in the process of collecting a comprehensive sample of 300-600 low- z Type Ia supernovae. Once such a sample is attained, we hope to perform spectroscopic analysis on obtained spectra and calibrate the results to further our understanding of Type Ia supernovae, their evolution, our standard candle use and the physics involved in their explosions. Often spectra are overpowered by Gaussian photon noise and corruption from cosmic rays and other natural phenomena. In order to analyze these spectra we face the constant challenge of finding a method to "denoise" them and highlight the spectral features for analysis. In this study, we explored wavelet analysis, which breaks down spectra into a diverse range of frequency components, by manipulating finite and localized base functions. Wavelet analysis employs many degrees of freedom, including choice of algorithm applied, number of scales used and format of reconstruction, allowing for a unique customization of spectral decomposition. We created noisy test spectra using the random number generator in the Interactive Data Language (IDL) and performed many statistical calculations to investigate the decomposition and placement of noise and signal. Additionally, we explored the reconstruction ability of wavelet analysis, performing systematic checks to ensure that primarily noise was removed in the spectral reconstruction. Finally, we tested the feature recovery ability of the wavelets and explored which scales highlighted the strong supernova spectral features. In future work, we hope to optimize the customization of wavelet use for the most accurate reconstruction and feature recovery results.

Spectroradiometer Calibration, Comparison, and Performance.

DANIEL STEEVER (University of Colorado, Boulder, Co 80301) DARYL MYERS (National Renewable Energy Laboratory, Golden, CO 89401).

Spectroradiometric measurements are key to quantifying the performance of spectrally sensitive photovoltaic (PV) devices. This project is an evaluation of the National Renewable Energy Laboratory's spectroradiometry systems. We identify sources of, and quantify measurement uncertainties among three spectroradiometers and make recommendations for improvement. Two spectroradiometers we tested (OL 750 and OL 754) were calibrated at temperatures between 20°C and 22°C. The third spectroradiometer tested, an LI-1800, was calibrated with a temperature-controlled detector at 20°C. All three spectroradiometers have an expected wavelength dependent measurement uncertainty ranging from $\pm 1\%$ to $\pm 4\%$. We tested the three spectroradiometers outdoors by making simultaneous solar irradiance measurements over a temperature range of 13.5°C to 24.7°C. We measured global horizontal, 40° tilt, global normal, and direct normal spectra. We analyzed the irradiance data for deviations between instruments exceeding the expected uncertainty limits. Deviations between the LI-1800 and the OL units were greater than $\pm 2\%$ in the 450-650 nm range. Irradiance differences increase with an increase in ambient and detector temperatures. We tested the LI-1800 performance with a commercial and a custom temperature control system using an environmental chamber and stable light source. Without auxiliary water cooling, thermal run-away occurred at 38°C. With the custom temperature controller, data at wavelengths below 1000 nm were within the range of expected variation, but data at wavelengths above 1000 nm were not.

3-Dimensional Atomic Resolution STEM. SAMUEL TRAVAGLINI (Harding University, Searcy, AR 72149) STEVE PENNYCOOK (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Currently, scanning transmission electron microscopes (STEM) create images that are projections of the crystalline structures being examined. Recent technical advances have allowed the spherical aberration (C_s) of the microscope, which causes rays traveling at different angles to be

focused differently, to be corrected. With the C_s fixed, the aperture angles for sending the beam in to the crystal have been allowed to grow, as they are no longer tied down to try and correct for the C_s . Given this technological advancement, the possibility of 3-D STEM image production has been explored using a multislice technique and comparing between simulations with and without phonons. Using a silicon crystal structure viewed down the direction with bismuth atoms attached in strategic locations on top of and within the silicon crystal, various focal series calculations were run. While also varying the aperture angles, an attempt was made to see if the image was able to resolve down to atomic resolutions in order to show exactly where an atom was located within a crystal. With the possible limitations that could be caused by channeling, heavier atoms were also studied. Using a CaTiO_3 crystal with La atoms embedded in it, similar simulations were run, and once again the results showed that as the aperture is widened and the probe size is diminished, the resolution begins to reach the atomic level, thus negating the effect that channeling has with the smaller apertures. The results seem to indicate that, given a wide enough aperture (> 100 mrad) and a small enough probe size ($\sim .05$ Angstrom) it is indeed possible to achieve atomic resolution in STEM imaging in 3 dimensions.

Development of a Diamond Powder Filter and 6H-SiC Monochromator for Triple-Axis Spectrometers. HAN-JONG CHIA (Grinnell College, Grinnell, IA 50112) STEPHEN E. NAGLER (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

Several materials were investigated as possible neutron optical devices for triple-axis spectrometers. Diamond powder was examined to determine its potential as a low energy band pass filter and single crystal Silicon Carbide explored to determine its viability as a monochromator. The ability of diamond powder to remove higher order neutrons of energy above 4.83 meV is undisputed. However, it exhibits low transmission of primary beam neutrons relative to cooled Beryllium. This is hypothesized to be due to small angle scattering arising from the voids between individual crystallites. Filling the voids with high neutron-scattering length density liquids was investigated as a method to mitigate the problem. Deuterated water was tested, but ultimately found to be ineffective since it lowered the transmission of neutrons compared to dry powder. At the time of this abstract's writing, Fomblin oil was being examined as a possible filler. Bragg scattering scans for a block of 6H-SiC showed it to have strong peak intensity in the (006) direction. Phonon scans for acoustic and optic modes were also performed on the crystal. The velocity of sound within the crystal was determined to be approximately 13,000 m/s. The Debye temperature was approximately 800 K. With verification of 6H-SiC's relative stiffness and knowledge that 6H-SiC has a large lattice spacing, future work can proceed to determine 6H-SiC's viability as a monochromator for triple-axis spectrometers.

Development of a Tune Setting Application for the Spallation Neutron Source Accumulator Ring. AMY LEAHMAN (Winston Salem State University, Winston Salem, NC 27043) SARAH COUSINEAU (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

The Spallation Neutron Source accumulator ring will use alternating sequences of quadrupole magnets to provide transverse focusing to the high intensity proton beam. The tune of the ring, defined as the number of phase space oscillations a particle undergoes in one ring revolution, is determined by the quadrupole strength settings. To manage the beam during operation, it is necessary to adjust the tune of the machine in each transverse plane. Therefore, the development of a user friendly software application for adjusting the tune of the machine is the primary task for this project. The application was developed using the Sun Java language within a standard XAL (Accelerator Library) framework, which provides menu bar and file manipulation tools. The application determines the quadrupole strength settings for the user requested tune point by interpolating from a grid of tune values and their corresponding quadrupole strength settings. Error percentages were calculated on the interpolation routine over the range of available tunes. Results indicate an error of less than 0.1% in most cases. However, the error increases significantly within $\pm 0.03\%$ of an integer value and reaches 100% when at the integer value 6.0. Additional focusing and defocusing adjustment tools were integrated to allow the operator the ability to fine-tune the quadrupole settings. The user also has the option to bypass the tune grid calculation and enter independent values for the quadrupole strength settings. The quadrupole strength set-points are sent to the machine via channel access; a read-back option is also available. A resonance tune plot has been added to visually portray the location of the tune point. Future plans for this application include a tune measurement capability, and connection of the program to the actual machine for further testing.

Effects and Correction of Closed Orbit-Deflecting Magnet Errors in the SNS Ring. STEVEN BUNCH (*University of Tennessee, Knoxville, TN 37996*) JEFF HOLMES (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

We consider the effect and correction of three types of orbit-deflecting errors in SNS: quadrupole displacement errors, dipole displacement errors, and dipole field errors. Using the ORBIT beam dynamics code, we focus on orbit deflection of a standard pencil beam and on beam losses in a high intensity injection simulation. We study the correction of these orbit-deflecting errors using the proposed system of 52 ring BPMs and an equal number of dipole corrector magnets. Correction is carried out numerically by adjusting the kick strengths of the dipole corrector magnets to minimize the sum of the squares of the BPM signals for the pencil beam. In addition to using the exact BPM signals as input to the correction algorithm, we also consider the effect of random BPM signal errors. For all three types of error and for perturbations of individual magnets, the correction algorithm always chooses the three-bump method to localize the orbit displacement to the region between the magnet and its adjacent correctors. The dipole corrector kick strengths obtained from correction of known errors can be used to set up a matrix which can be multiplied by arbitrary sets of magnet errors to obtain sets of kicks that agree closely with those obtained directly from the optimizer for those errors. When high intensity calculations are carried out to study beam losses, it is seen that the SNS orbit correction system, even with BPM uncertainties, is sufficient to correct losses to less than 10⁻⁴ in nearly all cases, even those for which uncorrected losses constitute a large portion of the beam.

Microstructure Analysis of Buffer Layers on Metal and Single Crystal Substrates by Atomic Force Microscopy (AFM). EMILY MILLER (*Juniata College, Huntingdon, PA 16652*) DAVE CHRISTEN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

In the Rolling-Assisted Biaxially Textured Substrate (RABiTS) approach to superconducting wires, YBa₂Cu₃O_{7-x} (YBCO) is grown upon buffer layers that have been deposited on metal substrates. Buffer layers provide barriers to separate the YBCO from the substrate. The YBCO films mimic the crystalline structure of the buffer layers and underlying substrates. Surface features such as grain boundaries and roughness of the buffer layers were studied. Buffer layers of La₂Zr₂O₇ and CeO₂ were deposited by physical vapor deposition and solution techniques onto Cu and Ni-based RABiTS. The surface characteristics of these buffer layers were analyzed by AFM. The surface morphologies of Yttria Stabilized Zirconia (YSZ) single crystal substrates having vicinal miscut angles of 0°, 4°, and 8° were investigated before and after annealing at a temperature of 1000°C in flowing oxygen. The results from these experiments revealed a direct relationship between an increase in the thickness of the films and an increase in the surface roughness. The method of deposition affects the surface roughness in such a way that the buffer layers applied to substrates through Electro Deposition have a higher surface roughness than layers grown by Radio Frequency Sputtering. A comparison between the grain boundaries of Ni-W and Cu shows similar behaviors. An analysis of non-miscut single crystal YSZ confirms the appearance of atomic level steps after annealing. By studying the surface morphology of buffer layers and substrates on which YBCO is grown, the effects of surface characteristics on the superconducting properties of the YBCO coatings can be determined.

Sequenced Symplectic Particle Transformations in Orbit. JOSHUA ABRAMS (*Knox College, Galesburg, IL 61401*) JEFFREY HOLMES (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

Ion beam behavior in accelerators is simulated via a computer code named ORBIT. This code follows user-defined particles as they traverse a lattice structure that describes the accelerator's influence. Building a lattice structure requires that the user assembles existing nodes that simulate real-world influences on actual ion beams. For example, a collimator node absorbs stray particles while a train of quadrupole nodes focuses an ion beam. Until now a formulation taken from the MAD computer program has been used to describe the nodes in our simulations. This formulation fails to satisfy an important property of Hamiltonian dynamics – symplecticity. As a result, MAD *single-particle transport* in ORBIT does not satisfy important properties of the Hamiltonian: non-linear phenomena, conservation laws, and long-term stability. Our group has created new nodes, which simulate particle-drifts, sector-bend magnets (dipole), primary-focusing magnets (quadrupole), and beam-correction magnets (sextupole, octupole and up), by means of sequencing symplectic particle transformations. These nodes incorporate all of the physics in the Hamiltonian while emulating element length; the latter is essential because real-world particles are affected throughout an element's length. Symplectic *hard-edge* (infinitesimally thin) fringe fields have also been added to the sector-bend and quadrupole nodes. Our

new nodes can either replace elements in an existing lattice structure or, given previous MAD parameters, serve as building blocks for an entirely new lattice.

Spectroscopic Exploration and Analysis of Spark Plug Erosion and Ignitability. SAMUEL GRAY (*Viginia Polytechnic Institute, Blacksburg, VA 24061*) JOHN WHEALTON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

This research is to determine how spark plugs break down and, from this information, to ultimately develop a diagnostic system that will be able to test an active spark plug and deduce how long it will be able to consistently create a spark before it breaks down. Each spark plug is tested by securely placing it within a pressure chamber, attaching to it one of two ignition systems, and then recording the spectrum of the light emitted by the spark. This is done by allowing the emitted light of the spark to be focused by a series of lenses onto the face a small diameter fiber optics cable. The light is then transmitted and projected into an optical spectrometer, where a camera captures a spectrum of each of the different sparks, as they are formed. With this setup many spark plugs can be tested, one at a time, while changes can be made to the amount of pressure within the chamber, the type of gas within the chamber, the type of ignition system being used, and the amount of light allowed to be collected and recorded as spectra. Through testing, it has been seen that as a spark plug ages eroded metal is projected into the gap, that the stability of the spark can be increased by removing this eroded metal that enters into the gap, that ignitability can be increased by incorporating a magnetic field in the spark, and that higher pressure increases the intensity of the spark.

Spectroscopic Exploration of Spark Plug Erosion. BENJAMIN HOSP (*Roanoke College, Salem, VA 24153*) JOHN WHEALTON (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*).

When voltage is sent to a spark plug in an engine, the voltage causes a spark in the gap at the end of the spark plug. When this spark occurs there is erosion at the site of the spark. Spark plug erosion is caused by several factors, including the material of the spark plug and the pressure of the surrounding gas. This erosion is studied by spectroscopic analysis of the light emitted by the sparks. Through study of sparks in several gases, including argon, nitrogen, and instrument air, it was possible to determine whether a certain line in the spectrum was caused by an interaction with the surrounding gas or gases or by the impact with the electrode. Extensive effort was applied to such attempts to categorize spectral lines. This allows for more direct quantification of erosion per spark. Certain new types of spark plug, particularly a Rotating Arc Sparkplug (RASP), are thought to cause less erosion than traditional spark plugs, as they more evenly distribute sparks across the electrodes. Also, there are continuing studies on the RASP dealing with design and erosion.

Using a Broadband Spectrometer and Spectra-Match Software to Increase the Efficiency of Laser Induced Breakdown Spectroscopy.

JOSHUA HARRISON (*Whitworth College, Spokane, WA 99251*) MAD-HAVI MARTIN (*Oak Ridge National Laboratory, Oak Ridge, TN 37831*). Laser Induced Breakdown Spectroscopy (LIBS) identifies a broad range of specimens based upon their individual elemental composition with great efficiency. While the size of the instruments decrease, the efficiency of LIBS processes increase, by utilizing new hardware capabilities, improving software operation procedures, and writing new software LIBS has become a more efficient means of element identification, which shall benefit research in a diversity of scientific fields. It is the purpose of this study to create new software in conjunction with improving the new broadband process, developed through varying levels of optimization, to acquire heightened levels of efficiency. The new broadband hardware is six times smaller than the old. The new process, in its current stage of development, collects data approximately 500 times faster than the old process. And it is estimated that the new data analysis software will analyze data 60 times faster than a researcher could do it manually. However the database upon which the newly created software relies needs further correction and investigation to improve the reliability of its analysis. Currently the new software can accurately identify seven specific elements in any mixture. In the future, pending more database research, this next generation of Spectra-Match software will be able to interpret data collected from the spectrometer and then display an element-composition of that sample freeing the researcher from unnecessary experimentation and data analysis by automating much of the LIBS process. The next progression for this software would be to begin with the element-composition then move to identify that subject based on its elemental composition using complex data libraries based upon existing researched matrices. One practical application for this technology would be for it to be able to identify archeological or crime scene remains giving inferences towards the subject's origin, species,

race or even dietary habits. This new process may one day shoot a bone fragment and tell the user that this bone came from a rabbit that foraged next to a contaminated stream. Current research will lead to the automation of: detecting counterfeit currency, identifying pollution, exploring micro films, sensing biohazards, conducting investigations in hazardous environments, processing rare-earth elements, producing actinides, and interpreting soil samples.

Characterizing the Performance of the Proton Transfer Ion Trap Mass Spectrometer. MATT NEWBURN (*Walla Walla College, College Place, WA 99324*) MICHAEL L. ALEXANDER (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The Proton Transfer Reaction Mass Spectrometer (PTR-MS) is technological innovation that is used to identify the components of gas mixtures and their concentrations. The PTR-MS is useful for analyzing gas mixtures because it allows for direct and real time monitoring. A second-generation instrument to the PTR-MS is the proton transfer reaction ion trap mass spectrometer PTR-ITMS. The advantages the PTR-ITMS has over the PTR-MS is that it has a higher duty cycle and allows for MS/MS analysis. In order for the results of the PTR-ITMS to be sensitive to trace gases the instruments settings must be optimized. The parameters that were varied are the low mass cutoff, collection time, drift tube pressure and the ion trap pressure because they are key factors to the sensitivity of the PTR-ITMS. This was accomplished by making sample mixtures of acetonitrile, acetone and benzene vapors in nitrogen gas. The goal of this study was to explore different methods for optimizing the PTR-ITMS. This study shows that there is not an apparent effect of the low cutoff mass to the sensitivity of the instrument. Also, it was found that varying collection time does affect the sensitivity of the PTR-ITMS, but the collection time could be significantly reduced in order to stop possible interferences from chemical ionization in the ion trap. This investigation shows the effects of Varying the drift tube pressure greatly affects the signal to noise ratio (SNR), at higher pressures the SNR decreases. Relative ion concentration is very dependent upon the pressure of the ion trap. This will allow great improvement over the previous settings. With these results second-generation PTR-ITMS will be an improvement upon the prototype instrument and even more so on that of the PTR-MS.

Growth and Characterization of Cu₂O films on MgO Single Crystals. JONATHAN ANDREASEN (*Illinois State University, Normal, IL 61790*) VAITHIYALINGAM SHUTTHANANDAN (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Cuprous Oxide (Cu₂O) powder has been shown to be a photo-catalyst and mechano-catalyst capable of efficient water splitting. The details concerning this process, however, are still unknown. By examining individual orientations of Cu₂O film, it may be possible to discover the underlying mechanisms of this reaction. We attempt to grow homogeneous Cu₂O thin films on an MgO single crystal substrate. We grow the film by vapor-deposition then characterize it using several methods including Rutherford Backscattering Spectroscopy (RBS), X-ray Photoelectron Spectroscopy (XPS), X-ray Diffraction (XRD), Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). We found the Cu₂O was grown along with Cu metal and that the film grew as islands while the chamber was backfilled with O₂ at a pressure of both 1 x 10⁻⁶ Torr and 5 x 10⁻⁶ Torr. Due to charging effects, we were unable to determine the ratio of Cu to Cu₂O in the film and thus could not resolve the exact composition of the islands or what lies between the islands in the film. We believe that a slower deposition rate will eliminate the presence of Cu metal on the surface.

Laser-Induced Damage of Calcium Fluoride. AUBREY ESPANA (*Washington State University, Pullman, WA 99163*) WAYNE P. HESS (*Pacific Northwest National Laboratory, Richland, WA 99352*).

As advances continue to be made in laser technology there is an increasing demand for materials that have high thresholds for laser-induced damage. Laser damage occurs when light is absorbed, creating defects in the crystal lattice. These defects can lead to the emission of atoms, ions and molecules from the sample. One specific field where laser damage is of serious concern is semiconductor lithography, which is beginning to use light at a wavelength of 157 nm. CaF₂ is a candidate material for use in this new generation of lithography. In order to prevent unnecessary damage of optical components, it is necessary to understand the mechanisms for laser damage and the factors that serve to enhance it. In this research we study various aspects of laser interactions with CaF₂, including impurity absorbance and various forms of damage caused by incident laser light. Ultraviolet (UV) laser light at 266 nm pulsing at femtosecond (fs) and nanosecond (ns) rates is used to induce ion and neutral particle emission from cleaved samples of CaF₂. The resulting mass spectra show significant differences suggesting that different mechanisms for desorption take place at each of these pulse

rates. Under irradiation of ns pulses at 266 nm single photon absorption is responsible for ion emission where as the fs case is driven by a multi-photon absorption process. This idea is further supported by the measurements made of the transmission and reflection of fs laser pulses at 266 nm, the results of which reveal a non-linear absorption process in effect at high incident intensities. In addition, the kinetic energy profiles of desorbed Ca and K contaminant atoms are different indicating that a different mechanism is responsible for their emission as well. Overall, these results show that purity plays a key role in desorption of atoms from CaF₂ when using ns pulses. On the other hand, once the irradiance reaches high levels, like that of the fs case, significant desorption is possible due to multi-photon absorption of the intrinsic material.

Study of the Measurement Variability in FTIR Spectroscopy Through the Characterization of a Nicolet Fourier Transform Infrared (FTIR) 710 Spectrometer. DAVID UNIMAN (*Santa Monica College, Santa Monica, Ca 90405*) NORMAN C. ANHEIER, JR. (*Pacific Northwest National Laboratory, Richland, WA 99352*).

The use of Infrared Spectroscopy for the identification of the chemical composition of unknown samples, especially carbon compounds, has proven an invaluable tool in various branches of science and technology. With the advent of FTIR spectroscopy, several advantages, such as an improved signal-to-noise ratio, a more efficient use of physical space, and a significantly reduced sampling time, were gained over its predecessor, Continuous Wave [diffraction] spectroscopy. Thus, we feel it is important to determine the measurement variability and study the possible sources of error in a standard laboratory FTIR spectrometer within the Near and Mid Infrared wavelength regions from 2.51 to 11.00 mm, in order to appreciate its accuracy and areas for improvement. Thermo-Nicolet v. 6.1a software was used to collect five data sets, each interpreted differently according to its area of analysis. The determination of the significance of random errors, the measurement variability per wavelength region due to such errors, as well as, a quantitative and qualitative analysis of the baseline drift as a function of time and wavelength region, were all interpreted from the data collected using standard and modified techniques. Error analysis showed that when the sample holder was removed and replaced, as opposed to remaining in a fixed position during the collection of a data set, the error (as measured at the 1s) increased by 0.1 %T throughout the studied wavelength regions. A modified sample/sample spectral analysis revealed the presence of bi-directional () ordinate errors due fluctuations in throughput strength from source to detector. The baseline drift was found to be linear with time per wavelength region. Baseline drift values of 0.420, 0.312, and 0.300 [%T/30 min between collected spectra] for 24 second scans in the wavelength regions of 2.90-4.00, 4.50-5.50, and 9.50-10.60 mm, respectively, were found. These values are within the manufacturer expected error margins of 0.75 [%T/1 min scanning time]; even more evident when the measurement variations previously found are taken into account. Despite the fact that the ordinate errors are bi-directional, the ability to place bounds on the measurement variability, as well as a significantly improved scanning time and S/N ratio, make FTIR spectroscopy a viable method for the analysis of unknown chemical samples, with great potential in numerous fields of study.

Synthesis and Characterization of Pure and Doped Ceria Films by Sol-gel and Sputtering. KURT KOCH (*University of Missouri-Rolla, Rolla, MO 65401*) LAXMIKANT SARAF (*Pacific Northwest National Laboratory, Richland, WA 99352*).

Pure and doped Ceria are known for their ability to gain or lose Oxygen, which is of interest to the Solid Oxide Fuel Cell (SOFC) and catalyst community. Current efforts are focused in SOFCs to reduce the operating temperature of the cell while maintaining ionic conduction. Ceria is known for its high ionic conductivity in the intermediate temperature region. (600-800° C) We have prepared pure and doped Ceria films by Sol-gel and magnetron sputtering methods. These films were characterized by X-ray diffraction (XRD), Rutherford backscattering (RBS), nuclear reaction analysis (NRA), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and Oxygen conduction measurements. We have observed greater volume diffusion in nanocrystalline Ceria compared to bulk polycrystalline films as a result of low density. Near surface diffusion properties indicate a decrease in the volume diffusion as a result of grain growth. However, a linear increase in O₂ content at 600nm depth was discovered and can be correlated to the redistribution of O₂ in the samples. Surface roughness of and oriented Ceria films on Al₂O₃ and YSZ was observed to be .13nm and .397nm, respectively. In the case of Ceria grown on YSZ, structural properties from XRD results showed a highly oriented structure with cube on cube growth. XRD results from Ceria grown on Al₂O₃ showed an oriented structure whose degree of orientation appeared to be partially dependent on substrate tempera-

ture. Preliminary XPS results indicate reduction in Ceria from the Ce⁴⁺ to Ce³⁺ state near the surface.

Ultrasonic Measurement of Light Liquid Viscosity. JUSTUS ADAMSON (*Brigham Young University, Provo, UT 84604*) MARGARET GREENWOOD (*Pacific Northwest National Laboratory, Richland, WA 99352*).

A method of measuring the viscosity of liquids is being researched at Pacific Northwest National Laboratory. This method provides an on-line measurement by measuring the density and the reflection coefficient of shear waves reflected off a surface of a known solid in contact with the liquid, which in turn yields the viscosity. Current research up to this point has been focused on defining and improving the consistency and sensitivity of the measuring technique by measuring the viscosity of water and sugar water samples. Results of this research have shown an accurate viscosity measurement is obtained immediately after calibration, but with a significant decrease in sensitivity over time. Possible improvements to the measurement system include change in wave path length, changes in electrical setup, and using an average water calibration. Future research should eventually lead to the capability of manufacturing commercially available pipeline or tank ultrasonic viscometers.

A Study of the Ortho and Para Visible Emission Line Intensities in a Helium DC Glow Discharge. LAURA BERZAK (*Dartmouth, Hanover, NH 03755*) ANDREW POST-ZWICKER (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

Although helium is a comparatively simple atom, its behavior as the working gas in a DC glow discharge is actually quite complex. Visible emission line intensities were studied as a function of pressure and axial position. The general peak intensity behavior correlated well to electron temperature, and the anomalous behavior of the 5875.6 Å peak, a 3³D to 2³P transition, was explained based upon level population mechanisms. The mechanism of most importance here is that of cascading, populating a level by de-excitation into it from a higher energy transition. This mechanism is not a significant factor in the singlet level populations. However, the same is not true for triplet levels, and the percentage of the 3³D level population due to cascading is a factor of at least three smaller than the contribution to all other observed triplet levels, thus accounting for the anomalous behavior.

Design of a Neutron Profile Diagnostic for the National Spherical Torus Experiment. ANDREW HERR (*Rensselaer Polytechnic Institute, Troy, NY 12180*) DOUGLASS DARROW (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

A time resolved radial profile neutron diagnostic is being designed for the National Spherical Torus Experiment (NSTX). The design goal is to achieve 5-7 cm radial resolution while minimizing the mass of the shielding. Experiments with a calibration neutron source have been performed to determine the dimensions and material composition of a collimating device needed to reduce cross-talk between channels and contributions from stray particles to acceptable levels. The well established MCNP transport code has been used to simulate attenuation and scattering. The laboratory experiment measuring attenuation through borated polyethylene, lead, and stainless steel has been simulated to determine optimal shielding around the detector. A model of a test collimator was produced, and the most effective dimensions for apertures was examined. Experimentally, the e-folding distance in borated polyethylene, the primary shielding candidate, was found to be 12 cm, but computer simulation found it to be 20 cm. Better agreement was found in the attenuation study where computer simulation correctly approximated the slope of the curve within a few percent. Best results were obtained from the simulation of the collimator when MCNP exactly mimicked experimental results. This result gives confidence in MCNP for future use. Much has been learned about materials and dimensions, so design of a neutron collimator can begin with more working knowledge as a guide.

Finite Element Computations of Magnetic Field Perturbations in a Tokamak Vacuum Region. EDWARD GORCENSKI (*Rensselaer Polytechnic Institute, Troy, NY 12180*) JON MENARD AND ALEXANDER PLETZER (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*). Understanding the dynamics of tearing modes in tokamaks is crucial as these modes can lead to the loss of plasma confinement. Previous numerical studies of tearing modes relied on approximating the conducting wall surrounding the plasma using a conformal geometry, i.e. an extrapolation of the plasma boundary by a constant factor. In contrast, the toroidal Laplace equation describing the magnetic perturbation in vacuum is solved, in this study, in a domain which can be irregular, such as the vacuum geometry on the National Spherical Torus Experiment.

The Development of an Experiment to Model the Potential Mathematical Correlation Between Ion Flux Across a Double Layer Structure in a Laboratory Plasma and Ion Flux Across an Organic Cell Membrane. EMILY HAMILTON (*Drew University, Madison, NJ 07940*) ANDREW POST-ZWICKER (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

The similar structures of a double layer formed in plasma and the biological cell membrane make the development of a mathematical model correlating the two a promising theoretical and experimental project. We use a stainless steel vacuum chamber with a wire mesh grid inserted in it acting as a secondary electrode to form the double layer sheath in the background plasma. Current versus voltage graphs were plotted to determine formation of the double layer, however chamber design fails to achieve necessary pressures for maintenance of a stable double layer. Future work will include more extensive probing of the plasma resulting in more accurate calculations, as well as chamber modification.

Torque Measurement and Ekman Effects in Taylor-Couette Flow. ROSS HAYS (*Northwestern University, Evanston, IL 60201*) HANTAO JI (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

Magnetorotational instabilities (MRI) are widely viewed to be a key angular-momentum transport mechanism in magnetized accretion discs; however, they have not yet been realized in a laboratory setting. An experiment, currently under way, will use liquid gallium to produce MRI in a Couette flow geometry. In order for MRI to be observed, it is necessary to have an accurate method of characterizing the fluid behavior and of differentiating between MRI-induced behavior and hydrodynamic behavior. One such method is to measure the fluid torque coupling between the inner and outer walls of a Couette flow. This coupling was observed by measuring the reaction torque exerted on the outer-cylinder driving-motor as both inner- and outer-cylinder rotation speeds were varied. This was performed alternately using air and water in the cell to establish mechanical and hydrodynamic background measurement methods for use in future MRI experiments. It was found that outward angular momentum flux and torque coupling were much stronger when inner-cylinder rotation rates were greater than the outer-cylinder rotation rates. Torque coupling measurements were compared with those expected for an Ekman-type transport mechanism based on hydrodynamic simulations.

Tritium Beta Imaging. JUSTIN LOPINA (*Beloit College, Beloit, WI 53511*) CHARLES GENTILE (*Princeton Plasma Physics Laboratory, Princeton, NJ 08543*).

Tritium, a component of fusion fuel, emits beta radiation with a half-life of approximately 12.5 years. An isotope of hydrogen, Tritium, which has a 100% beta decay, is a small molecule and therefore difficult to contain and detect. Utilizing a CCD camera under appropriate conditions, tritium and tritium-contaminated materials can be observed through phosphor interaction. A plate of phosphor is placed above the tritium sample in an environment void of external light. Over a period of 60 to 200 seconds, the CCD camera will collect photons from the tritium-excited phosphor. Difficulties involve appropriate focusing, light pollution, and slight background radiation. This technique may prove useful by providing a reliable way to detect surface tritium, as well as identifying its exact location and relative strength of radioactivity. This paper will describe the imaging configurations, including test results and applications.

A Comparison of the Availability and Failure Modes of the BaBar Superconducting Solenoid with Similar Magnets at Other High Energy Physics Laboratories. MALLORY KNODEL (*Drake University, Des Moines, Ia 50311*) J. G. WEISEND II (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

One of the key technologies in the BaBar detector is the 1.5 T superconducting solenoid. It is imperative that this device operate reliably at its nominal current to allow data taking. While this system is available for physics 98.8% of the time, further improvements are desirable. The object of this project is to survey similar magnet systems, for example those at KEK (Belle), Fermilab (D0 and CDF), DESY (H1 and ZEUS), and CERN (ALEPH and DELPHI), to see how often such magnets stop functioning properly and what the root causes of the failures are. A survey was carried out via e-mail and telephone calls. Information was obtained regarding the operation of superconducting magnets, specifically the BaBar magnet and its ancillary systems, as well as an overview of the use of other such magnets both in the US and overseas. In this work, failure modes will be investigated and compared to the BaBar operational experience. Future investigations can now assess the feasibility of reducing the time the BaBar magnet is nonoperational and unavailable for physics research.

BaBar Instrumented Flux Return Replacement Research and Development. MELISSA BERRY (Baker University, Baldwin City, KS 66006) PETER KIM (Stanford Linear Accelerator Center, Stanford, CA 94025). The Instrumented Flux Return (IFR) of the BaBar detector will soon need to be replaced by a more robust muon detection system. Scintillator bars with embedded Wavelength Shifting (WLS) fibers and Limited Streamer Tubes are two replacement technology options. The scintillator bars are tested for attenuation length; and causes for the large width of the Photo Multiplier Tube (PMT) signal are analyzed by Monte Carlo simulation. Cooling techniques for Avalanche Photo Diodes (APD) are investigated. The fairly high attenuation length coupled with the narrow PMT signal make the scintillator a viable option for a muon detecting system. Continuing work will focus on increasing timing resolution using an APD to read the signal from the WLS fibers, and investigating the lifetime of the APD. The ability to read a signal from the LST on external copper strips is tested and signals are found to be clearly distinguishable from noise. The voltage is compared to count rate to find that the optimal operating voltage for the LST used is 4600V. Further studies will be conducted in strip readout and fabrication as well as in the optimal isobutane content in the gas mixture that flows through the tube.

Beam-Beam Interactions. CHRISTOPHER SRAMEK (Rice University, Houston, TX 77005) TOR RAUBENHEIMER (Stanford Linear Accelerator Center, Stanford, CA 94025).

At the interaction point of a particle accelerator, various phenomena occur which are known as beam-beam effects. Incident bunches of electrons (or positrons) experience strong electromagnetic fields from the opposing bunches, which leads to electron deflection, beamstrahlung and the creation of electron/positron pairs and hadrons due to two-photon exchange. In addition, the beams experience a 'pinch effect' which focuses each beam and results in either a reduction or expansion of their vertical size. Finally, if a beam's disruption parameter is too large, the beam can develop a sinusoidal distortion, or two-stream (kink) instability. This project simulated and studied these effects as they relate to luminosity, deflection angles and energy loss in order to optimize beam parameters for the Next Linear Collider (NLC). Using the simulation program Guinea-Pig, luminosity, deflection angle and beam energy data was acquired for different levels of beam offset and distortion. Standard deflection curves and luminosity plots agreed with theoretical models but also made clear the difficulties of e-e- feedback. Simulations emphasizing kink instability in modulated and straight beam collisions followed qualitative behavioral predictions and roughly fit recent analytic calculations. Finally, a study of e-e- collisions under design constraints for the NLC provided new estimates of how luminosity, beamstrahlung energy loss, epsilon parameter and deflection curve width scale with beam spotsizes.

Characterization of E-158 Beam. JOE FARRELL (San Francisco State University, San Francisco, CA 94110) JIM TURNER (Stanford Linear Accelerator Center, Stanford, CA 94025).

Stanford Linear Accelerator Center (SLAC) parity violation experiment E-158 uses a high intensity electron beam accelerated to either 45GeV or 48GeV in the SLAC Linac and requires a small energy spread, small off axis position motion, and low jitter. The purpose of our research was to better quantify the current values of energy, intensity, and position jitter as well as the relations between them and to further the understanding of the beam dynamics involved. Specifically, our method was to take data on a series of pulse lengths shorter than the experimental beam to gain information about the length dependence of the different beam parameters, effectively enabling us to create jitter, position, and energy profiles of the beam. Position was measured by beam position monitors (BPMs), intensity was measured by toroids, and energy was measured by a Synchrotron Light Monitor (SLM) as well as several energy BPMs. Data was collected using the SLAC Control Program (SCP) and analyzed using MATLAB. Position jitter was found to, in general, increase linearly (10microns per 50ns) with pulse length. The peak to peak energy difference across each pulse is currently about 0.4% of the total energy, with the RMS energy jitter usually ranging from 0.013% to 0.10% for the different pulse lengths. Intensity jitter had no discernable correlation with pulse length. The slope of the linear relation between energy and intensity (beam loading relation) varied significantly with pulse length as well as with the method used to extract energy data. The position, intensity and energy profile data agree qualitatively with accepted theories and provide a more encompassing picture of the beam dynamics for E-158. The same is true, to a lesser extent, for the energy jitter and beam loading data, although some results here were unexpected.

CRAnE: A JAS-based Data Acquisition System for Cosmic Rays. JENNIFER DOCKTOR (North Dakota State University, Fargo, ND 58105) TOM GLANZMAN (Stanford Linear Accelerator Center, Stan-

ford, CA 94025).

Cosmic Ray Analysis Environment (CRAnE) is a software tool designed to collect and plot data from a cosmic ray telescope (CRT) connected to a computer serial port. As a plug-in to Java Analysis Studio (JAS), CRAnE provides visual displays of incoming cosmic ray rates as they are detected. In an effort to make the program user-friendly, it operates through a graphical user interface. This paper describes the features of CRAnE and includes installation and operation instructions in the appended user's manual.

Decision Tree Technique for Particle Identification. RYAN QUILLER (Rensselaer Polytechnic Institute, Troy, NY 12180) CHARLES C. YOUNG (Stanford Linear Accelerator Center, Stanford, CA 94025).

Particle identification based on measurements such as the Cerenkov angle, momentum, and the rate of energy loss per unit distance ($-dE/dx$) is fundamental to the BaBar detector for particle physics experiments. It is particularly important to separate the charged forms of kaons and pions. Currently, the Neural Net, an algorithm based on mapping input variables to an output variable using hidden variables as intermediaries, is one of the primary tools used for identification. In this study, a decision tree classification technique implemented in the computer program, CART, was investigated and compared to the Neural Net over the range of momenta, 0.25 GeV/c to 5.0 GeV/c. For a given subinterval of momentum, three decision trees were made using different sets of input variables. The sensitivity and specificity were calculated for varying kaon acceptance thresholds. This data was used to plot Receiver Operating Characteristic curves (ROC curves) to compare the performance of the classification methods. Also, input variables used in constructing the decision trees were analyzed. It was found that the Neural Net was a significant contributor to decision trees using dE/dx and the Cerenkov angle as inputs. Furthermore, the Neural Net had poorer performance than the decision tree technique, but tended to improve decision tree performance when used as an input variable. These results suggest that the decision tree technique using Neural Net input may possibly increase accuracy of particle identification in BaBar.

Distinguishing Photons from Muons using the Time-over-threshold in the Tracker from the Gamma Ray Large Area Space Telescope.

RENATA RAWLINGS (Florida A&M University, Tallahassee, Florida 32301) EDUARDO DO COUTO E SILVA (Stanford Linear Accelerator Center, Stanford, CA 94025).

The Gamma Ray Large Area Space Telescope, GLAST, is a large scientific instrument designed to study gamma ray activity in space. GLAST is designed to detect gamma rays with greater energy and angular resolution than previously done by gamma ray telescopes. A portion of GLAST is the Large Area Space Telescope (LAT), which is made up of sixteen identical towers encased in an anticoincidence detector. The source of the data for this study is a simulation of one of these towers. The LAT will detect gamma rays by using a technique known as pair-conversion. When a gamma ray slams into a layer of tungsten in the tower it creates a pair of subatomic particles (an electron and its anti-matter counterpart, a positron). Where this pair hits the detector has an effect on the photon's signal distribution. When a specific series of cuts are done a difference in the gamma ray signal as compared to the background signal is seen. This shape difference will ideally be the crux of detecting gamma rays. This study is a small portion of the total preparations done to enhance the gamma ray signal coming into the detector.

Evaluation of the Electronic Bubbler Gas Monitoring System for High Flow in the BaBar Detector. ANGELA LITTLE (Seattle Pacific University, Seattle, WA 98119) KELIN WANG (Stanford Linear Accelerator Center, Stanford, CA 94025).

We evaluated the gas monitoring system in the Instrumented Flux Return (IFR) portion of the BaBar detector at the Stanford Linear Accelerator Center (SLAC) to determine its suitability for flows greater than 80 cc/min. Future modifications to the IFR involve particle detectors with a higher gas flow rate than currently in use. Therefore, the bubbler system was tested to determine if it can handle high flow rates. Flow rates between 80 and 240 cc/min were analyzed through short term calibration and long term stability tests. The bubbler system was found to be reliable for flow rates between 80 and 160 cc/min. For flow rates between 200 and 240 cc/min, electronic instabilities known as baseline spikes caused a 10-20% error in the bubble rate. An upgrade would be recommended for use of the bubbler system at these flow rates. Since the planned changes in the IFR will require a maximum flow of 150 cc/min, the bubbler system can sufficiently handle the new gas flow rates.

Gamma Ray Large Area Space Telescope Event Analysis: An Examination of Events Recorded by the LAT Prototype Detector. JASON HEIMANN (University of California, Santa Cruz, Santa Cruz, CA

95064) **EDUARDO DO COUTO E SILVA** (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

The GLAST mission requires an orbiting satellite that will detect and analyze gamma rays from distant cosmic sources. A prototype particle detector (called the minitower) has been built: a scaled-down model similar to that which will be used in the satellite. Previous experiments using the prototype detector have provided cosmic ray data taken at different signal thresholds. These data were processed with a track reconstruction algorithm that performed interpolations to approximate the path that each particle traveled. Using ROOT, we produced many graphs of the data to characterize the detector's response to cosmic rays and find correlations within the data. The coordinate system used in the data was verified against specifications and sensitive areas of the detector were measured. We have validated the geometry implementation of the detector using cosmic ray data, studied hit multiplicity and its angular dependence, and examined detector response under different threshold settings. A basic understanding of the detector's characteristics has been developed for future investigation of charge sharing between strips.

Mapping of Ambient Magnetic Fields within Liquid Helium Dewar for Testing of a DC SQUID Magnetometer. **RANDAL NEWHOUSE** (*Whitworth, Spokane, WA 99251*) **DAVID FRYBERGER** (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

In an effort to explore the cavity lights phenomenon, Experimental Facilities Department at SLAC is testing a DC SQUID magnetometer. Due to the nature of the SQUID magnetometer and the intended tests, the earth's magnetic field must be negated. It is proposed to reduce ambient fields using bucking coils. First, however, an accurate map of the magnetic field inside the liquid helium Dewar where the experiment is going to take place needed to be made. This map was made using a three-axis fluxgate magnetometer mounted on a 3D positioning device made for this purpose. A ten inch tall volume within the Dewar was measured at data points approximately an inch from each other in all three axes. A LabVIEW program took readings from the magnetometer at 2 ms intervals for 1000 readings in such a way as to eliminate any ambient 60 Hz signals that may be present in the data. This data was stored in spreadsheet format and was analyzed to determine how the magnetic field within the Dewar was changing as a function of position.

Mass Profile of Abell 2204. **TRAVIS LAU** (*University of Central Florida, Orlando, FL 32816*) **GREG MADEJSKI** (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

The vast majority of the matter in the universe is of an unknown type. This matter is called dark matter by astronomers. The dark matter manifests itself only through gravitational interaction and is otherwise undetectable. The distribution of this matter in can be better understood by studying the mass profile of galaxy clusters. The X-ray emissions of the galaxy cluster Abell 2204 were analyzed using archived data from the XMM-Newton space telescope. We analyze a 40ks observation of Abell 2204 and present a radial temperature and radial mass profile based on hydrostatic equilibrium calculations.

Missing Mass Recoiling Against the Charged D^{*}: Monte Carlo Based Investigation of a BaBar Recoil Peak at 2620 MeV. **HILLARY CAIN** (*Dartmouth College, Hanover, NH 03755*) **ART SNYDER AND STEVE WAGNER** (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

This paper chronicles the investigation of a peak in the BaBar mass data set of mass recoiling against charged D^{*}s. Our hypothesis is that the peak at 2620 MeV is a reflection of the Ds^{*} and pion system. Specifically, we explored the idea that the peak might be a reflection from the decay B goes to D^{**} Ds⁺ with the D^{**} goes to D^{*} pion. Theoretically, when the D^{**} decays, the trajectory of the resulting pion will form an angle with the Ds⁺, and different angles impart difference masses to the system over a range of a GeV or so. If quantum mechanics dictates that their paths will form a particular angle more often than others, a peak would appear in the histogram of their collective mass. Using the Monte Carlo model of particle collision events, Anders Ryd's EVTGEN program, C++ code derived from GeneratorsQA, and PAW, we tested the hypothesis that the peak might be a reflection of the system, but found that this possible explanation could not account for the peak. No 2620 MeV peak appears in the histogram of the system mass. We therefore discount the hypothesis and conclude that some other reflection, statistical fluctuation, or particle is causing the peak.

Modeling the Transverse Linear Optics of a Charged Particle Storage Ring. **PHILIP TANEDO** (*Stanford University, Stanford, CA 94309*) **YITON YAN** (*Stanford Linear Accelerator Center, Stanford, CA 94025*). Charged particle storage rings play a key role in the frontiers of high-energy physics. For the most part, however, particle physics is largely

unaccessible to undergraduate-level students, discouraging such students from taking an early interest in it. It is our premise, however, that the fundamental physics of storage rings can, in fact, be taught at this stage, fostering interest in accelerator physics. In this paper we present an introduction to the transverse linear optics of a charged particle storage ring suitable for second-year undergraduates. We begin by introducing transverse motion in the one-dimensional case to establish a familiarity with linear lattices. We then move on to our primary goal which is to analytically decompose a coupled two-dimensional system with a minimal amount of axiomatic treatment (the derivation of the decoupling matrix, for example). While this is by no means a comprehensive exposition on beam dynamics, it serves to provide meaningful insight into the fundamental physics involved in these machines for introductory students. It is our hope that this approach can be extended to other aspects of high-energy physics so that undergraduates may have a better glimpse at the frontiers of their field.

Parameterized Shower Simulation in Lelaps: A Comparison with Geant4. **DANIEL BIRT** (*California Institute of Technology, Pasadena, CA 91125*) **AMY NICHOLSON** (*New York University, New York, NY 10010*) **WILLY LANGEVELD, DENNIS WRIGHT** (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

The detector simulation toolkit Lelaps simulates electromagnetic and hadronic showers in calorimetric detector elements of high-energy particle detectors using a parameterization based on the algorithms originally developed by Grindhammer and Peters and Bock et al. The primary motivations of the present paper are to verify the implementation of the parameterization, to explore regions of energy where the parameterization is valid and to serve as a basis for further improvement of the algorithm. To this end, we compared the Lelaps simulation to a detailed simulation provided by Geant4. A number of different calorimeters, both electromagnetic and hadronic, were implemented in both programs. Longitudinal and radial shower profiles and their fluctuations were obtained from Geant4 over a wide energy range and compared with those obtained from Lelaps. Generally the longitudinal shower profiles are found to be in good agreement in a large part of the energy range, with poorer results at energies below about 300 MeV. Radial profiles agree well in homogeneous detectors, but are somewhat deficient in segmented ones. These deficiencies are discussed.

Q-switching the Flash Ti:Sapphire Laser. **KELLY CONE** (*California Polytechnic State University, San Luis Obispo, CA 93401*) **AXEL BRACHMANN** (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

The Stanford Linear Accelerator Center (SLAC) uses a flash lamp pumped Ti:Sapphire laser to generate the electron beam inside of the Linac. This laser system was installed at the SLAC Polarized Light Source in 1993. During the past, the system has been upgraded in several steps (eg. installation of Rhodium coated reflectors, cavity redesign, and remote controlled wavelength tunability). Q-switching the laser cavity to increase the peak pulse energy was successfully investigated and further improves the capabilities of the laser system for future polarized beam experiments. Two Pockels cells were used to perform the Q-switch and various diagnostics were used to characterize the modified laser pulse. The timing in relation to the laser trigger, pulse width, and pulse shape applied to the Q-switching Pockels cells (PC) were optimized. No damage to the laser cavity or optical elements occurred. At optimal conditions of Q-switching, the pulse energy of the laser increased from 0.4 mJ to over 3 mJ in a 300 ns pulse. The Q-switched pulse energy can be further increased by extending the hold-off pulse applied to the PC. The laser pulse produced by the Q-switch was long enough {full width half maximum (FWHM) > 200 ns} for pulse shaping and demonstrated good intensity stability (< 0.5% jitter). The increase in output power suggests that Q-switching will be used for future accelerator projects.

Solving the Neutrino Mass Mystery Using Double Beta Decay. An Examination of the Feasibility of Xenon Purification and Ion Capture and Release Using an Electrostatic Probe. **VERENA MARTINEZ OUTSCHOORN** (*Harvard University, Cambridge, MA 02138*) **PETER C. ROWSON** (*Stanford Linear Accelerator Center, Stanford, CA 94025*). Double beta decay has long been recognized as a useful avenue for the study of electron neutrinos, especially the neutrino mass and its fundamental nature (Majorana or Dirac). Recent neutrino oscillation experiments have provided compelling evidence that the neutrino has mass. The detection of the neutrinoless mode of double beta decay would finally set a lower limit on the mass of the electron neutrino, as well as prove that the neutrino is a Majorana particle (with opposite spin, it is its own anti-particle). The Enriched Xenon Observatory (EXO) project attempts to detect neutrinoless double beta decay using ¹³⁶Xe that decays by this process to ¹³⁶Ba⁺⁺ + e⁻ + e⁻. Perhaps one of the most

significant characteristics of this project is the reduction of the background through the identification of the Barium ions for each individual event using laser fluorescence techniques. This project also proposes to collect scintillation light in addition to the ionization electrons in order to further improve energy resolution. Current work at SLAC includes the development of a purification system for xenon, as well as tests for the capture and release of single ions using an electrostatic probe.

The Effects of Mechanical Hardness on Radio Frequency Breakdown. KRISTI ADAMSON (*Brigham Young University, Provo, UT 84604*) STEFANIE HARVEY (*Stanford Linear Accelerator Center, Stanford, CA 94025*).

Preliminary high-energy tests have been performed on the next linear collider test accelerator and the traveling wave structures have been examined with a scanning electron microscope. This has yielded the locations of radio frequency breakdowns, characterized by surface craters, occurring on the oxygen-free electric copper traveling wave structure. It has been proposed that the occurrence of high voltage breakdown may be related to material hardness. We have examined this possibility by measuring the hardness of various crystal grains within the copper structure and searching for any correlations to the breakdown events. The hardness of various copper crystal grains has been measured with a nano-indenter and the crystal grains have subsequently been analyzed for breakdown damage. This preliminary analysis does not show any explicit indications that mechanical hardness may be related on the occurrence of RF breakdown. Further research is suggested to verify these initial results.

Analysis of Positron Rates for Hall C Experiment 94-110. TANYA OSTAPENKO (*Gettysburg College, Gettysburg, PA 17325*) ROLF ENT (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

One result of an inelastic electron-nucleon collision is the production of electron-positron pairs. The pair-produced electrons cannot be distinguished from electrons directly scattered from the target nuclei. Such pair-produced e^- contaminate the data and the e^- cross section. In order to compensate for pair production in the calculation of the e^- cross section, the ratio $1-(e^+ / e^-)$ displays the factor by which the e^- yield must be reduced in the final total number of scattered e^- . This ratio will be examined for hydrogen target runs at varying beam energies, angles and momenta.

Application of Wavelet Methods to Relativistic Scattering and Bound States of the Gross Equation. BRIAN KESSLER (*University of Iowa, Iowa City, IA 52242*) J. WALLACE VAN ORDEN (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

For scattering energies typical at Jefferson Lab, a non-relativistic description of nucleon interactions is inadequate. The Gross (spectator) equation provides a relativistically covariant description of nucleon interactions in terms of momentum space integral equations. Unfortunately, a properly symmetrized formulation of this equation results in a potential term with spurious moving singularities. Traditional solution techniques have difficulty dealing with this numerical problem. Numerical methods employing a wavelet basis have shown promise at being able to deal with this type of isolated structure in a controlled and efficient manner using the discrete wavelet transform (DWT). The DWT produces a sparse representation that decreases solution time without sacrificing accuracy by isolating relevant structures. In the context of a simple scalar model, we developed and applied wavelet techniques to solve for the coupling constant from the bound state and to produce the two-body scattering matrix. The code was implemented in FORTRAN and analyzed for stability and speed of solution. Though the results are ambiguous, some of the methods presented may prove useful in future calculations.

Calibration of Constant Fraction Discriminators (CFDs) and Development of Cryostat Exit Detector (CED) System for the G0 Parity Experiment. KRISTIN KIRILUK (*University of Maryland, College Park, MD 20742*) GARY RUTLEDGE (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

The G0 experiment will study the contribution of strange quarks to the proton's electromagnetic properties using parity violating electron scattering. The experiment has two modes of operation: at forward angles, the protons are detected, and in the backward angle mode the electrons are detected. The detector is an array of scintillation counters and photomultiplier tubes, whose signals are digitized with Constant Fraction Discriminators (CFDs). The backward angle mode requires the addition of Cryostat Exit Detectors (CEDs) and Aerogel Cerenkov counters to distinguish electrons from pions. The construction and assembly of a prototype CED/Aerogel module was carried out to identify and fix mechanical interferences and to develop and test a lightweight

support system. This included designing and machining mounts for the phototubes for the CEDs as well as building a prototype Cerenkov assembly. From the construction of the prototype, several interference issues have been identified and fixed. In addition to construction of the prototype CED/Aerogel module, a program was developed to calibrate the effective threshold voltage for the CFDs and to check their reproducibility with varying input pulse widths and shapes. It was determined that the CFD modules show a small difference in effective threshold voltage when comparing the square pulse data to the photomultiplier tube (PMT) signal data. The CFD modules yield reproducible results when subjected to varying pulse widths.

Cosmic Testing of the BigBite Spectrometer. CHARLES HANRETTY (*Florida A&M University, Tallahassee, FL 32307*) DOUGLAS HIGINBOTHAM (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

In order to increase the experimental capabilities of Jefferson Lab's Hall A, the construction of a third spectrometer called BigBite is underway. This spectrometer is a "third arm" for the experimental hall and will provide data complementary to that collected by the High Resolution Spectrometers. In preparation for BigBite's use in Hall A, the detector package needed to be cabled and the Data Acquisition System (DAQ) needed to be tested. Signal and high voltage cables were made, tested, and connected to both the detectors and the DAQ. By using cosmic rays, the detector package and the DAQ was tested. The data gathered from this testing was used to generate the position and angular distribution spectrums of cosmic rays passing through the detector package. The BigBite detector package has been completed, tested, and is now ready for installation and use in Hall A.

Event Analysis using the Graphical Event Display in Jefferson Lab Hall A's ROOT/C++ Analyzer. ROBERT STRINGER (*California State University Los Angeles, Los Angeles, CA 90032*) OLE HANSEN (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

In order to investigate problems with and improve the accuracy of the track reconstruction algorithm used in the new ROOT-based C++ analysis software under development in Hall A at Jefferson Lab, a new tool was required, that would allow detailed examination of individual events. To accomplish these tasks a Graphical Event Display was created. The GED provides a 3-D view of the High Resolution Spectrometers and displays hits in the VDC, reconstructed tracks, paddles on the scintillators, and active blocks in the shower counters on an event-by-event basis. The track y position at each active scintillator paddle is calculated on timing data from the PMTs. The GED also presents detail views of the Vertical Drift Chambers showing the cluster fitting and track reconstruction. This model allows for quick identification of incorrectly reconstructed tracks and detailed analysis of individual events. Using the GED to analyze data from experiment E01-012 at Jefferson Lab we saw a relatively large number (42%) of single VDC wires receiving multiple hits. The majority these secondary hits may occur due to intermittent ionization as the particle passes through the VDC, resulting in discrete pulses being registered on the wires. The track projection y-position at scintillator S1 with the y position determined from timing data we saw a correlation with an uncertainty of $\delta = 0.06$ m, which is consistent with the uncertainty of the scintillator timing measurement. The analysis of events using the GED can lead to improvements in the methodology used in software track reconstruction and will be a useful tool in Hall A's analysis software.

High Energy Neutron Detectors for Thomas Jefferson National Accelerator Facility (TJNAF) experiment E-02-013 (GEN) . NATHAN HUDSON (*Kent State University, Kent, OH 44242*) BOGDAN WOJTSKHOWSKI (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

Virtually no data exists about the neutron electric form factor G_E^n at high Q^2 . Due to the fact that the net charge of the neutron is zero, G_E^n is small at low Q^2 . Because free neutron targets on which experiments can be performed do not exist, TJNAF experiment 02-013 will collide electrons with a ^3He target to produce recoil neutrons. By analyzing the scattering of the recoil neutrons, data about neutron electric form factor can be obtained. An array of 5 layers of plastic scintillators bars will detect the neutrons. Each bar will be attached to two photomultiplier tubes (PMT's), one on each end. The scintillating material will be highly polished for maximum internal reflection and covered in aluminized Mylar to reflect any stray photons back into the bars. Strips of black plastic will protect the Mylar and provide light isolation, and electrical tape will cover the corners of the square bars to absorb ambient photons. An acrylic light guide will connect the scintillating material to the photomultiplier tube. Each PMT will be housed in an aluminum cylinder, sealed by thermoshinking rubber and an O-ring to prevent light and air leaks. A hole in the top of the housing will allow the atmosphere

inside to be regulated to ensure a low concentration of helium to avoid tube damage. A cylinder made of m-metal, an iron and nickel alloy, will provide magnetic shielding for the photomultiplier tubes. Finally, after assembly and a set of efficiency tests, all the bars will be ready to serve as neutron detectors for GEN.

Moller Polarimetry Systematics in Hall C. *CRYSTAL BERTONCINI (Vassar College, Poughkeepsie, NY 12604) DAVID GASKELL (Thomas Jefferson National Accelerator Facility, Newport News, VA 23606).* Some experiments, especially those studying weak interactions, need to know the polarization of the beam to a high precision, and the Hall C Moller Polarimeter at Thomas Jefferson National Accelerator Facility (TJNAF) is well equipped to offer such high precision measurements. To get the best measurement possible, it is best to know what affects the polarization measurement. First, data already collected from some previous experiments were used to test for correlations of polarization with parameters such as beam current, raw event rate, leakage current, and more. Then, an analytical function that describes the magnetic field of the solenoid in the Moller Polarimeter was fit to a field map. After inserting this function in the Moller Monte Carlo, the simulation was used to test the effects of solenoid misalignment and beam energy with respect to analyzing power. Reassuringly, all the systematic tests had little effect on polarization. Of all of the correlations tested, the only possible correlation found was between polarization and charge asymmetry — for one subset of the data, the chi-squared per degree of freedom for charge asymmetry improved from 1.701 at a constant fit to 1.505 at a straight-line fit for Wein angle 60.2 degrees and from 3.211 to 2.670 at 71.2 degrees. This could be attributed to the limitations of the equipment used in the beam current measurement. For the solenoid field, a piecewise function fit to within within 3.23787% for Bz and 14.815% for Br, corresponding to deviations of at most 0.13201 T and 0.015257 T respectively at a nominal 4T field. Also, misalignment of the solenoid up to 6.000 mm in x and y and 0.006 radians in dx' and dy' had at most a 0.83102% effect on the analyzing power with less than a 1% uncertainty. A study of varying beam energies from 1-6 GeV using several different solenoid models similarly resulted in no real dependence between polarization and beam energy. In conclusion, the measured polarization has no correlation with the range of systematic effects tested, except for charge asymmetry, which may simply require further calibration of the Beam Current Monitors (BCM's).

Self-chirped Pulse Compression in the Free Electron Laser. *BRIAN GLOVER (University of Central Florida, Orlando, FL 32803) STEPHEN BENSON (Thomas Jefferson National Accelerator Facility, Newport News, VA 23606).*

In the superradiant regime of the Free Electron Laser (FEL) the Japan Atomic Energy Research Institute (JAERI) has recently found and published numerical evidence of pulse compression using self-chirp compensation. A general property of the FEL superradiant pulse is its inherent nonlinear frequency chirp due to radiation emission at down-shifted frequencies. JAERI showed that pulse compression could lead to a temporal duration as short as two optical cycles (FWHM). This nonlinear chirp has been found numerically at the Thomas Jefferson National Accelerator Facility (TJNAF). We show numerical evidence of pulse compression to a width below two optical cycles for the TJNAF's IR UPGRADE FEL oscillator. Numerical compression of the UV DEMO is also presented and discussed. A two grating compression system is designed and presented for the IR UPGRADE oscillator.

SCIENCE POLICY

Optimizing Efficiency Standard Levels for Distribution Transformer Design Lines with Life Cycle Cost and National Impacts. *MATTHEW WINKLER (Williams College, Williamstown, MA 01267) JOHN STOOPS (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*

The Energy Policy Act of 1992 mandates an energy efficiency standard for distribution transformers. Due to the millions of distribution transformers in use in the United States, even small gains in efficiency could mean large gains in monetary and energy savings as well as environmental benefits. Life Cycle Cost (LCC) analysis for distribution transformers is an important step in deducing such possible national impacts of the proposed efficiency standard. The LCC analysis which analyzes the initial cost plus usage costs over the lifetime of a transformer looks at five proposed efficiency levels compared to a baseline, non-standard level. The first level corresponds to an industry defined standard level. The fifth level corresponds to the engineering maximum. This project assessed the intermediate levels and searched for new efficiency levels that yield the greatest LCC savings over the baseline level. It also looked at the utility and necessity of searching for new efficiency levels to an accuracy of .01%. It was found that significant behavior in the

LCC savings curve was missed when only the initial Candidate Standard Levels were used. It was also found that optimizing existing levels for LCC savings created an interesting scenario with a high net present value (NPV) of savings while still maintaining large energy savings. New efficiency levels inputted for design lines 5 and 9 had noticeable effects on national impacts but more work is needed to understand how much impacts new levels would have for all design lines.

Proposal for Installing Grid-Connected Renewable Hybrid Systems on the Kalaupapa Peninsula of Molokai, Hawaii. *REBECCA HALL (CU-Boulder, Boulder, CO 80501) OTTO VAN GEET (National Renewable Energy Laboratory, Golden, CO 89401).*

The Kalaupapa Peninsula is located on the north side of Molokai Island, Hawaii. The village of Kalaupapa was initially established as a colony for sufferers of Hansen's disease, but today it is a National Historical Park, operated by the National Park Service (NPS). Currently the village receives electricity from the main grid on Molokai, which connects to the village via lines dropping over 2000-foot sea cliffs. Degradation of the electric lines and maintenance difficulties have led the park to consider establishing renewable energy systems to cut their energy costs for three systems: new trash incinerators, water pumps and village electrical power. The National Park Service (NPS) has enlisted the help of the Federal Energy Management Program (FEMP) to investigate these three systems. FEMP used the Hybrid Optimization Model for Electric Renewables (HOMER), a modeling program developed at NREL for designing renewable hybrid systems, to find feasible solutions for reducing the park's energy costs. The NPS proposes an aggressive recycling program and, based on HOMER simulations, the installation of a 900 W trash incinerator powered by a 600 W PV array with a 48 V battery bank. Currently, a 100 kW generator powers a water-pump to deliver 65,000 gallons of water per day (GPD), which is a load of 166 kWh/day. FEMP proposes decreasing water usage to 30,000 GPD, requiring a load of 77 kWh/day. Since transportation of diesel fuel to the remote water pump site is difficult and dangerous, FEMP proposes the installation of a World Water Solar Pumping System. The current electric load for the village is 3.3 MWh/day. This includes the electricity needs of 40 Hansen's patients, 30 health-care workers including a hospital, and 30 park employees. As the NPS will most likely wait to install renewable energy until after the patients have all left the village, this proposal assumes a daily load of 0.817-1.634 MWh/day. The peninsula has a good wind resource, with annual average wind speeds of 7 m/s. At 1.634 MWh/day, FEMP recommends installing one FL-100 turbine or two AOC-15/50 turbines connected to the grid. At a load of 0.817 MWh/day, FEMP recommends installing one AOC-15/50 turbine connected to the grid. Although there is currently no net metering through the Maui Electric Company, the village's current supplier, the wind turbines will offset the electric costs by up to 15% over the next 25 years.

Oak Ridge National Laboratory's Influence on Location of the Technology Industry. *JUSTICE GRAHAM (University of Tennessee, Knoxville, TN 38572) TERRY PAYNE (Oak Ridge National Laboratory, Oak Ridge, TN 37831).*

Oak Ridge National Laboratory's (ORNLs) Economic Development division creates and assists businesses in the technology industry with federal and state assistance programs (e.g. funding, research). In order to calculate its impact on this region, a study was done to discover how many technology-related businesses have operations in a three county area adjacent to the lab (Blount, Anderson, and Knox). The more information that can be retrieved about these businesses, the better Economic Development would be able to assist them. In order to gather information, the State chamber was contacted and asked if they could provide info on all businesses in Tennessee with certain North American Industry Classification System (NAICS) codes. This classification system is used in order to compare statistical data about businesses across North America. Then lists of company names (from mailing lists and user agreement lists) were gathered from Technology 2020 and Economic Development. After filtering unwanted data, and researching for further information, the lists were combined. After gaining contact information, a website was made to host a survey. Businesses were then contacted and linked to the website where they could provide the information requested by ORNL. The business information was then compiled into a working database. A map was also plotted to clearly depict the concentration of businesses in the three county area. Results and conclusions have yet to be defined because the website was just recently finished and there have been no significant changes in the data.

Assessment of the 2003 Energy Bill in Relation to the Office of Science. *LAUREN CIALONE (Butler University, Indianapolis, IN 46208) JACK BAGLEY (Pacific Northwest National Laboratory, Richland, WA 99352).*

Legislation within the Office of Science section of the Energy Bill is critical, due to the affect its authorizations have on physical science research conducted there. In assessing the Office of Science language of the Energy Bill, it is important to examine both the bill passed by the House of Representatives as well as that of the Senate. The House bill (H.R.6) was passed April 11th of this year; however the Senate voted to abandon its bill (S.14) and pass H.R.6 with an amendment in the form of a substitution that contained last year's bill from the 107th Congress (H.R.4), which never made it out of conference. Issues and programs within the Office of Science portion of the bill include Fusion Energy, Spallation Neutron Source, Nanotechnology, Genomes to Life, Catalysis Research and Computing. With respect to the two bills pending in conference several of the authorizations made by both the House and Senate are significantly similar, if not identical. However when the old Senate bill, H.R.4 is compared with S.14, which had been moving forward since the spring, it evidently lacks allocations in several segments of the bill. When Congress returns in September, the Republican controlled both House and Senate will conference at the Senate. It is expected that despite the complications encountered in the production of S.14, Senator Pete Domenici (R-NM), sponsor of the bill, will bring forth legislation from S.14 in conference.

Safety. RHONDA BUTTS (*Saint Augustine's College, Raleigh, NC 27610*) GAYLE SUNDEEN-COLEMAN (*Thomas Jefferson National Accelerator Facility, Newport News, VA 23606*).

Safety in the workplace is an issue that is dealt with on a daily basis. Everyone in the workplace has to be knowledgeable of common and uncommon work hazards in order to have a safe working environment. In the engineering group at Thomas Jefferson National Accelerator Facility (TJNAF), concerns such as electrical and machine safety are just a few important safety factors to be aware of. Workers must be aware of the types of hazards involved and take precaution when handling electrical equipment or machinery. Being well informed of the safety procedures, manufacturer's recommendations, and the risks involved will significantly reduce the amount of injuries that occur when handling machinery, electrical, or a lockout/tagout procedure.

WASTE MANAGEMENT

Polychlorodibenzo-p-dioxin and Polychlorodibenzo-furan Removal and Destruction. STAVAN PATEL (*Santa Monica College, Santa Monica, CA 90405*) MICHAEL KAMINSKI (*Argonne National Laboratory, Argonne, IL 60439*).

Polychlorinated dibenzo-p-dioxins (dioxins) and polychlorinated dibenzo-p-furans have been generated as unwanted by products in many industrial processes. The dioxin isomer 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) has been called the most toxic compound known to man. In this paper a review of destruction and removal technologies for dioxins and furans are reported. Also, proposed ways of removing dioxins using magnetic nano-particles are reported.

Waste Form Development Samples for Immobilization of Mixed Waste. MATTHEW RODRIQUEZ (*University of Idaho, Moscow, ID 83843*) ROY GRANT (*Argonne National Laboratory, Argonne, IL 60439*).

Treatment and the disposal of mixed waste is necessary in such a manner that if not treated properly may cause extreme danger to the environment, also affecting most organisms. Something can be categorized as mixed waste if it is radioactive and hazardous (chemically). Argonne National Laboratory operates Treatment, Storage, and Disposal facilities used to treat mixed waste. To guarantee the mixed waste be treated and disposed of properly the Resource Conservation Recovery Act (RCRA) has regulations that are mandatory for this to happen. RCRA provides the list of characteristics identifying whether something is a hazardous waste. Also, RCRA states the regulated levels for disposal of a mixed waste. Radioactivity is regulated by the Department of Energy (DOE). Turco 4502 is a waste stream currently being stored at the INEEL and considered for treatment at Argonne National Lab-West. The waste stored is a mixed waste requiring treatment and disposal. The EPA codes for this product are D001 and D007. D001 is the characteristic of ignitability (oxidizer). D007 is the characteristic of chromium; the level of chrome has to be greater than or equal to 5mg/L to be considered hazardous. The mixed waste is an oxidizer from potassium hydroxide and is also hazardous from potassium chromate. Turco 4502 is a product made up of KOH, $KMnO_4$, and K_2CrO_4 . A surrogate was created instead of using the product to minimize exposure to the radiation associated with the drums in which the product is stored. Treatment would consist of a way to neutralize the KOH, and stabilize the chromium to Land Disposal Restriction (LDR) standards. The LDR standards are that

the chromium needs to leach from the waste at less than .6mg/L TCLP in order to dispose of the waste. The method used was not successful; I believe it was due to the conversions made to reduce the oxidation state of CrVI to CrIII. More testing will consist of adding additional ferric sulfate to try and reduce the oxidation state of chromium six to a three so it does not leach as easily. This is what seems to be the biggest factor for successfully treating the mixed waste.

System Dynamics. LISA MAYO (*Brigham Young University - Idaho, Rexburg, ID 83460*) VANESSA NELSON (*Brigham Young University - Idaho, Rexburg, ID 83440*) JAKE JACOBSON (*Idaho National Engineering & Environmental Laboratory, Idaho Falls, ID 83415*).

Typically, as engineers build waste barrier caps, they account for static elements and fail to consider many of the dynamic elements. Due to these overlooked elements, 146 of 163 caps tested by the Environmental Protection Agency (EPA) have led to ground water contamination. The scientists and engineers at the Idaho National Engineering and Environmental Laboratory (INEEL) are building a model applying system dynamics to better understand the dynamic processes that affect a caps performance. This knowledge will enable us to build longer lasting, self-healing, and less expensive evapo-transpiration (ET) caps that can be applied to waste sites around the nation. System dynamics is an analytical approach that examines systems by studying their underlying structure. Doing so allows us to make predictions relative to how the system will react to change. Due to the many changing variables in nature, this cap model is indeed complex; however, system dynamics helps observers predict how different environmental changes such as: droughts, floods, and fires will change the cap's performance. The ability to test different soil types and precipitation rates allows engineers and scientists to design an ET cap that will work best in their climate. Software programs, Stella® and Vensim®, provide a method for modeling and simulating this data. Through this software, we have compiled the components of the ET cap model into a chart, which displays the linear connections among the components. This chart presents a clear visual not only for team members and those interested in the ET cap, but also for those interested in system dynamic models. The key to system dynamics is understanding that any system is better than the sum of the parts.