BIOLOGY

Purification and Crystallization of Proteins. *LOUR-EVELYN O. LEZONDRA (Northern Illinois University, Dekalb, IL 60115) NUKRI SANISHVILI and IRINA DEMENTIEVA (Argonne National Laboratory, Argonne IL 60439).*

Protein structures offer not only visual representations of macromolecules, but also serve as a link to understanding the functions they generate and how they can be manipulated. Structures are derived from x-ray diffraction patterns produced by an x-ray beam through a protein crystal. However, the formation of crystals must be preceded by various methods for protein isolation and purification. Translation of target protein DNA into E. Coli allows the desired protein to increase in quantity through the cell replication. The cells are then harvested and lysed to release the target protein. Furthermore, several purification steps are rendered to isolate the protein: filtration, nickel chromatography, dialysis, concentration and Thrombin cleavage. Each step extracts contaminants that may hinder the formation of good quality crystals. After purification, which yields about 1ml of protein solution, crystallization screens are performed to optimize growing conditions. Attempts at purification and crystallization PG 31 (Molybdopterin Biosynthesis Protein from E.Coli) were successful, yielding a fairly large crystal of good quality. However, PG 33 (Biotin Synthase from E.Coli) did not crystallize. Instead, it produced salt crystals that originated from the buffer. Finally, the remainder of the proteins PG 35 (Biotin Synthase from H. Influenzae), PG 36 (Aminotransferase from E. Coli) and PG 41 (Aminotransferase from H. Influenzae) became insoluble during dialysis. The latter results indicate possible alterations in buffer content since crystal formation by proteins are extremely vulnerable to pH, temperature, certain salts, etc.

Purification and Crystallization of E2A-HLF and HLF(N) Constructs for X-Ray Crystallography. *MAYA EVERETT (St. Mary's College of California, Moraga, California, 94575) G. McDermott (Lawrence Berkeley National Laboratory, 94720).*

Understanding how proteins function is an essential part of biology. Proteins control almost every chemical reaction within the cell. Their function is a direct result of their structure. Determining their structure uncovers insight into how the protein works. The principle method for determining protein structure is by x-ray crystallography. In this experiment, the crystallization process of protein constructs E2A-HLF and HLF(N) was initiated for the purpose of x-ray crystallography. These constructs are part of the protein E2A-HLF found in patients with acute B-form leukemia. Discovering the structure may lead to information on how the protein works and insight regarding the disease. *E. coli* were used to synthesize the protein tagged with GST. The protein was separated via glutathione column and the GST tag removed. The protein solution was concentrated and initial conditions were set-up to explore different crystallization possibilities. Although the E2A-HLF construct became insoluble after lysing of the GST tag, the HLF(N) construct was successfully purified and different crystallization conditions initiated.

DNA-based characterization of MTBE biodegrading microbial communities. *Arlene Rivera (Universidad Metropolitana, Rio Piedras, Puerto Rico, 00928) Dominique C. Joyner and Tamas Torok (E.O. Lawrence Berkeley National Laboratory, Berkeley, California 94720)*

A quantitative molecular technique, terminal restriction fragments length polymorphism (T-RFLP), was utilized for rapid analysis of microbial community diversity in various environments. In this study we compared fluidized bed reactor (FBR) microbial community diversity in two methyl tertiary butyl ether (MTBE) bioreactors and two enrichment cultures from the FBR. The 16S rRNA from total community DNA was amplified using polymerase chain reaction (PCR) in which one of the two primers used was fluorecently labeled at the 5'end. The amplified 16S rRNA was digested with restriction enzymes creating different size fluorescent-labeled terminal restriction fragment which were separated by electrophoresis using an automated DNA sequencer. Ten samples were screened by using T-RFLP the results show community shifts over time with unique peaks specific to the different sampling times. A partial DNA sequence was determined for one clone, Iso a 2, using primers 27f, 926f and 907r. The strain was identified as *Desovia riboflavina*. Overall, our results demonstrate that T-RFLP and DNA sequencing are powerful tools for assessing both the diversity of complex microbial communities and identifying individual that comprises the communities.

Whole Genome Shotgun Sequencing *Author: Waterhouse, En. DOE Lab: Lawrence Berkeley Lab, Berkeley, CA.*

Whole Genome Shotgun Sequencing involves randomly cutting many copies of an organism's DNA into pieces that are small enough to be sequenced, and then laterally developing the DNA's structure by looking for similarities between the sequenced pieces. Dr. Dan Rokhsar's group, in conjunction with members of NERSC's Scientific Computing Group led by Dr. Esmond Ng, is developing their own Whole-Genome Shotgun Assembly algorithm. The goal of this project is to develop an assembler that is optimized for parallel supercomputers and more quickly and accurately completes genome assembly than current algorithms. This paper presents the results of two background studies for this project. First, a literature review on DNA repeats is presented. Secondly, the composition of three sets of read sequences from the Joint Genome Institute's mouse sequencing project is analyzed. We find that the average probability of a single base occurring is 0.270 ± 0.006 for A, 0.245 ± 0.004 for T, 0.240 ± 0.004 for G, 0.244 ± 0.004 for T, and 0.002 ± 0.0005 for N, indicating a slight overpopulation of A's in the reads. We also find that that N's are much more likely (at minimum a factor of 10) to be found near single base repeats than they are to appear alone. This trend grows with the size of the repeat. We also find that N's are clustered at the tips of the reads, with the highest concentration at the end where sequencing is terminated

Evaluating Corn Stover Hydrolyzate Toxicity. *GARY MCMILLEN (Community College of Southern Nevada, North Las Vegas, NV 89030). NANCY DOWE (National Renewable Energy Laboratory, Golden, CO 89401).*

Lignocellulosic materials offer a cost-effective way to produce ethanol from biomass. These materials include sawdust, herbaceous grasses, agricultural residues, and waste paper. Before these materials can be fermented to ethanol by microorganisms, they must be pretreated with dilute acid under heat. The liquid that results from this pretreatment is known as hydrolyzate. The hydrolyzate contains sugars that can be fermented by microorganisms. Unfortunately, the hydrolyzate may also be quite toxic to the microorganisms. Thus, the hydrolyzate needs conditioning and is usually conditioned through ion exchange and overliming. Corn Stover offers hope as a cost-effective lignocellulosic feedstock because it may contain less of the toxins that many of the other hydrolyzates contain. Thus, the focus of the current study is to evaluate the toxicity of non-overlimed and overlimed hydrolyzate using the bacterium *Zymomonas mobilis* and the yeast *Saccharomyces cerevisiae* in shake flask and fermentation experiments. Results of the experiments indicate that raising the pH of the corn stover hydrolyzate to facilitate organism growth is the only conditioning that the stover needs. Thus, corn stover may help lower productions costs for ethanol due to its low toxicity.

Fermentation Broth Rheology, Assay for Cellulase Enzyme Production, and Continuous Batch Substrate Addition. *Ronald D. Kloberdanz (Colorado State University, Fort Collins, CO, USA 80521) K. Kadam (National Renewable Energy Laboratory, Alternative Fuels User Facility, Golden, CO 80401-3393).*

Due to shortages and reliance on foreign sources of petroleum, and environmental concerns from the burning of fossil fuels, the National Renewable Energy Laboratory is researching production of ethanol from lignocellulosic biomass material. One aspect of this research is production of enzymes that are used to hydrolyze the cellulose into glucose for subsequent fermentation to ethanol. The goal of this project was to develop new techniques that will enhance enzyme production research. A new assay was implemented to measure one of the major enzyme components (endo-1,4-?-glucanase). Fermentation viscosity was also measured and modeled to gain further knowledge on enzyme broth rheology. This is important for design and scale-up of production systems. Another part of the project was the installation of a fed-batch feeding apparatus on a 15-L fermentor. Fed-batching decreases the

need to overload substrate at the fermentation start, and may improve some of the rheological problems. This system was tested and shows promise for future application.

Sounding Healthy: The Virtual Human's Need for Speed; Parallelizing Computational Fluid Dynamics Code. *Todd L. Miller (Haverford College, Haverford, PA) Kara L. Kruse (Oak Ridge National Laboratory, Oak Ridge, TN) Dr. Richard C. Ward (Oak Ridge National Laboratory, Oak Ridge, TN)*
The Virtual Human project connects three-dimensional anatomical and dynamic physiological models of the human body to investigate a wide range of biological and physical responses to various stimuli. As part of the Virtual Human project, computational fluid dynamics — numerical approximations of the response of fluids to forces — is used to model generation of lung sounds. Lung sounds in the middle airways of healthy people are produced primarily by complex vortex flow due to the multiple curved branchings of the airways. Because of the accurate data, complex geometry, and requirement for fine details in the fluid flow, the current simulation code ('PHI3D', developed at Oak Ridge National Laboratory by Dr. Paul T. Williams) runs unacceptably slowly. The parallelization of the finite-element basis matrix formulation used custom-developed codes and MPI, and succeeded in reducing run time approximately one-third in the best case. Replacing the matrix equation solvers with the PETSc parallel package (developed by Argonne National Laboratory) unexpectedly caused the code to run twelve times slower . Explanations and future directions are detailed.

Oxidative Enzyme Reaction in Organic Mixtures. *DALEIK A. VAUGHN (Tuskegee University, Tuskegee, AL, 36088) Dr. BRIAN H. DAVISON (Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37830).*
Until the late 1980's, the scientific community as a whole had a general perception that enzymes only work in aqueous solutions. Recently there has been research that liberates the idea of enzymatic reactions only occurring in aqueous solutions. The analysis of enzymatic reactions in organic solutions is now of interest. Enzymatic reactions occurring in organic media are being studied for several reasons. It is believed that, if active, enzymes are more stable in organic solution and product recovery from organic solutions will be inexpensive. In addition, new reactions may be possible. Most nonaqueous enzymes have been hydrolases; we are beginning to utilize oxidases in organic mixtures. Many oxidative enzyme reactions require a steady but small amount of hydrogen peroxide. However, an excess of hydrogen peroxide will cause the enzyme to become inactive. The challenge is to determine how to provide the steady but small amount of hydrogen peroxide in order to carry out the reaction. It was known that when glucose is mixed with glucose oxidase (GOX), hydrogen peroxide is produced. Chloroperoxidase (CPO) is the enzyme that is under investigation in these experiments. CPO's and GOX's activities were tested in mixtures of aqueous buffer with two organic solutions, acetonitrile or acetone (0-70%). GOX or CPO's initial rate activity in organic solutions was measured using standard dye reactions, and spectrophotometry. A mixture of CPO and GOX will ultimately be used to epoxidize aromatics such as styrene or alkenes such as octene.

The Use of Peroxidases in Enzymatic Fuel Production. *APRIL S. WARREN (Middle Tennessee State University, Murfreesboro, TN, 37130) Tanya Kuritz (Oak Ridge National Laboratory Oak Ridge, Tennessee 37830).*
The need for cheaper fuel prompted the Lignin Peroxidase Project. Lignin is found naturally in trees, and the enzyme lignin peroxidase (LiP) from the fungus *Phaneracheate chrysosporium* breaks lignin down. The LiP may also break down aromatic rings in petroleum, which would convert high molecular weight aromatic hydrocarbons into molecules usable as fuel. This conversion would decrease the price of gasoline production from petroleum. This enzyme is important because it can also be used to degrade other substances and ultimately use them for fuel sources. In order to develop such a biotechnological hydrocarbon conversion system, we need to produce sufficient amounts of active enzyme. Our strategy involved the expression of the gene encoding LiP from *P. chrysosporium* in easily propagatable yeast. The *lip* gene was introduced to the yeast *Pichia pastoris* by genetic engineering for this purpose. Recombinant yeast were screened for enzyme activity and generation of the data for the analysis of the process kinetics. The recombinant cultures were sampled daily and tested using a spectrometer for the presence of the enzyme. A total of seven recombinant strains were tested and some were promising for further investigation. This experiment could have major effects on the fuel industry in the coming years.

Plant Genetics, New Frontier Breakthroughs. *Author: Chambers, DOE LAB: PPNL*
Plant genetics is the new frontier for scientific breakthroughs. Work in this area can result in benefits for widely diverse areas, conserve energy, conserve environments, reduce waste, and promote cost efficiency. Plant cell transformation and promoters are particularly significant areas of plant genetics. Promoters are necessary for the success of foreign gene regulation and plant cell transformation. In our experiments, the behavior of two different promoters used by plant genetic engineers, rpl34 which controls a cytoplasmic ribosomal protein with a high homology to the rat 60S r-protein L34 (Gao et.al., 1994) and Mac, a promoter hybrid that includes the CaMV35S and Ti plasmid mannopine synthetase (mas) promoters (Comai et. al., 1990)—were closely monitored. We transformed plant cell cultures using *Agrobacterium* that contained plasmids with a bacterial beta-glucuronidase (GUS) gene under the control of rpl34 and Mac promoters. The GUS gene was chosen as a marker gene, which is an acid hydrolase that catalyzes the cleavage of the substrate 4-methylumbelliferyl B-D-Glucuronide or MUG, to release a fluorescent compound, methylumbelliferyl. Thus, during the analysis, GUS expression and activity can be measured by the increase in fluorescence. Transformed plant callus cultures were screened and GUS expression in transformed suspension cultures was monitored. Results show that as protein increases, total GUS activity increases. Further, as protein increases, GUS specific activity decreases but remains constant after the first day. Also, biomass, extractable soluble protein, and total GUS concentration reach a peak after four days of culture.

Targeted Gene Deletion in *Shewanella Oneidensas* MR-1. *Jamie Elizabeth Lemus (Truckee Meadows Community College, Reno, Nevada, USA 89506) M. Romine Ph.D. (Pacific Northwest National Laboratory, Richland, Washington 99352).*
Shewanella oneidensis strain MR- I is able to use iron and other multivalent metals as terminal electron acceptors during respiration. The consequent reduction of metals by this metabolic process results in significant changes in metal solubility, either greater or less depending on the element. For some radio-nuclides, such as U and Te, microbial reduction results in the precipitation of relatively insoluble metal oxides, thereby limiting their mobility in aquifers where they can pose a health risk. Our goal is to identify the genes encoding proteins important to this process. A protein called TatC is necessary for mobilizing many respiratory proteins into the membrane. If they are not mobilized there they will not work. To determine if TatC mobilizes the iron reductase in Shewanella, we propose to delete the tatc gene from the genome. If the deletion mutant is not able to respire iron we can infer that one of the few protein (-IS) mobilized by this protein is the iron reductase.

Studying the Photosynthetic Apparatus of The Purple Non-sulphor Bacteria *R. capsulotis* and *R. sphaeroidies*. *David G. Mets (University of Rochester, Rochester, NY 14627) Dr. Deborah K. Hanson and Dr. Philip D. Lible (Argonne National Laboratory, Argonne, IL 60439)*
The research discussed in this paper covers three separate topics. Due to the type of paper presented here, and the requirement that it cover a time period and not a specific topic, these topics will be discussed in clearly defined sections, starting with the abstracts. These sections are:
1. Wrong Way Electron Transfer in Purple Photosynthetic Bacteria, as Induced by Protein Engineering Within *Rhodobacter sphaeroidies* 2. Effects of Oxygenation Levels Upon LH2 Expression Within *Rhodobacter sphaeroidies* 3. Isolation and Crystalization of LH1/RC Superasemblies from *Rhodobacter capsilotis 1. Reaction Center Mutagenesis* Electron transfer within the reaction centers of wild-type purple non-sulphor photosynthetic bacterium occurs primarily down the A-side of the chemically symetrical two branch system. The reason for that singular direction of transfer, however, is not known. Induction of B-side transfer through site directed mutagenesis of the protein residues surrounding these chemical chains is the goal of this project. These residue changes may also affect the overall structure of the protein. These changes are also important to observe. These mutated reaction centers will be analyzed through the use of UV/VIS/near IR spectroscopy, time resolve ultra

fast spectroscopy, EPR spectroscopy, and X-ray crystal diffraction. *2. LH2 Optimization* Light harvesting antennae type II (LHII) of purple non-sulphor photosynthetic bacterium are controlled by an elaborate regulation mechanism which is clearly affected by the oxygen concentration of the given culture. The extent to which this oxygenation regulation system affects the production of plasmid born LHII is investigated in these experiments. Varying levels of oxgenation in cultures of both plasmid born LHII as well as wild-type cells were grown up and the levels of LHII in both sets of cultures were determined. It is clear that the deletion strain and the wild-type do not exhibit the same control, possibly because the plasmid is missing much upstream and downstream DNA that is contained on the chromosome. *3. Super-Assembly Isolation* The structure of the LHI has not been determined with a high level of precision. The nature of the interaction between the LHI complex and the reaction centers of purple non-sulphor photosynthetic bacterium has not been determined. Through the isolation and crystallization of the LHI, reaction center super-assembly would allow detailed modeling of the LHI complex as well as the interaction between the LHI complex and the reaction centers. Currently the vapor diffusion crystal trials are still equilibrating.

Functional Analysis of Plant Promoter rpL34 Using the *GUS* Marker Gene in New Tr,tnsgene Expression Vector pZD428. *Jacqueline Mauzey-Amato, (Truckee Meadows Community College, Reno, Nevada 89512). Ziyu Dai, Ph.D, (Pacific Northwest National Laboratory, Richland, WA 99355).*

Optimization of the transgene expression system is one of the critical steps for the high level production of heterologous proteins in plants, where the promoter is a key component regulating transgene expression. In this study, the activity of the *rpL34* promoter was analyzed in transgenic tobacco *(Nicotiana tabacum)* NTI calli. A DNA fragment containing the *rpL34* promoter
and the reporter gene B-D-glucuronidase (GUS) were cloned into binary vector pZD427 to generate the transgene expression vector pZD428. The insertion was verified by enzyme restriction digestion and agarose gel electrophoresis analyses. The DNA fragment containing the *rpL34* promoter and *GUS* reporter gene was then integrated into the tobacco genomes via *Agrobacterium funiefaciens-mediated* NT] suspension cell transformation. The transformed CaNi were induced on Murashige and Skoog (MS) plates containing proper amounts of 2,4-D, cefotoxime, and kanamycin. Two hundred and sixty transformed calli were harvested for GUS activity and protein concentration measurements. GUS activity analyses revealed the specific activity up to 278,358 units per milligram total soluble protein. The GUS activity under the control of the *rpL34* promoter is much higher than that under the control of the cauliflower mosaic virus 35S promoter, a commonly used promoter in plant biology. These results suggest that the *rpL34* promoter is one of the most active promoters that can be used for heterologous protein production in calli and suspension cells.

The Use of PIT Tagging to Estimate Juvenile Fall Chinook Salmon Migration Time Through the Priest Rapids Project Area on the Columbia River. *REBECCA WAHL (Lewis and Clark College) Geoffrey McMichael (Pacific Northwest National Laboratories, Richland, WA 99352)*

We are in the process of evaluating how the Priest Rapids Project (PRP, located north of the Hanford reach on the Columbia River) affects populations of wild, fall Chinook salmon that are produced. One part of this project involves using mark-recapture technique to monitor fall juvenile Chinook movement in the area. A passive integrated transponder (PIT) tag technology was used to document migration timing out of the influence of the PRP, and track fish through downstream dams as they make their way to the ocean. On June 6 and 7, 2000, we tagged 1083 fall Chinook sub-yearlings above and below Wanapum Dam, subsequently detecting them as they began to pass through downstream dams. As of 9 August 2000, 122 fish had been detected in one or more of the dams downstream of the PRP. A mean migration time for tagged the fish of 5.5 km/day below the McNary dam and 4.5 km/day above the McNary Dam. The mean migration rate between McNary Dam and John Day Dam was 21.4 km/day. Back calculation, indicated the mean date of departure for juveniles tagged in the pool above Wanapum Dam was July 16, 2000, while juveniles tagged below Wanapum Dam was July 1, 2000. Because fish are still being detected at the dams only preliminary conclusions can be attempted. Since the peak of migration time for these fish seems to have passed, the time when these fish most likely left the PRP area can also be estimated. Data analysis will continue analysis, and hopefully some of the adult returns will be measured as they come through the dams throughout the duration of the project.

Exploring the Photosynthetic Reaction Center and Light Harvesting Antennae of *Rhodobacter capsulatus* and *Rhodobacter sphaeroides*. *ZACHARY S. MORRIS (Ripon College, Ripon, WI 54971) Dr. Philip D. Laible and Dr. Deborah K. Hanson (Argonne National Laboratory, Argonne, IL 60439)*

The summer ERULF fellowship research I pursued under the guidance of Dr. Philip D. Laible and Dr. Deborah K. Hanson entailed three primary projects that were supplemented on occasion with smaller extraneous projects. The focus of this paper is the three central projects upon which my research efforts were concentrated. Each section of this paper will be divided into three sections (to be labeled as 1. Mutagenesis 2. Oxygenation 3. Super-assemblies) as is appropriate for the discussion of three separate projects. 1. *Mutagenesis* Induction of B-Side Electron Transport in Photosynthetic Reaction Centers of *Rhodobacter sphaeroides* by Site-Directed Mutagenesis. While it is known that electron transport in wild-type reaction centers of purple photosynthetic bacteria occurs unidirectionally down the A-side of the complex, it is not known why this uniform direction of transfer exists. In an attempt to observe high yields of B-side electron transport in the reaction centers of *R. sphaeroides*, site specific mutations were made in the L gene. In addition to our intended mutant strains, additional mutations were achieved due to possible inconsistencies in the PCR-based method we utilized for amplification of site-directed mutagenized plasmids. Reaction centers of each of our mutants, including those unintentionally created, have been purified and are currently being studied by UV spectroscopy, EPR, and x-ray crystallography. 2. *Oxygenation* Qualitative Analysis of Oxygen and Light Level Effects on LHII production in *Rhodobacter sphaeroides* Light Harvesting antennae type II (LHII) are known to be the primary receptors of electromagnetic energy in the process of photosynthesis within *R. sphaeroides.* These antennae are known to be produced and degraded in response to varying levels of oxygenation and light as is appropriate for the metabolic needs of the cell and the capacity of the reaction center to convert excited state energy into electron transport. Studies were done on the effects of oxygen and light on LHII production in the wild-type and in a strain carrying a plasmid-borne *puc* operon. While our data agree with previous studies of LHII transcriptional controls, our results are preliminary and at this point must be viewed as qualitative rather than quantitative. These strongly suggest that the plasmid-borne LHII lacks certain transcriptional controls. From these tests we have made generalizations regarding LHII production optimization in wild type and the strain carrying the plasmid borne *puc* operon. Such information may prove useful in proposed cloning reactions. 3. *Super-assemblies* Solubilization, Purification, and Crystallization of LHI/RC Super-assemblies from *Rhodobacter sphaeroides* and *Rhodobacter capsulatus* Despite advances in the technology of x-ray diffraction, the structure of LHI and the nature of interaction between LHI and the reaction centers of both *R. sphaeroides* and *R. capsulatus* remain unknown. In addition to this, the reaction center of *R. capsulatus* is yet to have been crystallized in a manner suitable for diffraction. We have developed and optimized techniques for the solubilization of wild-type super-assemblies (reaction centers bound by LHI) from both *R. sphaeroides* and *R. capsulatus* by use of a mild detergent. Solubilized super-assemblies were purified by affinity chromatography, concentrated by centrifugation, and put into crystallization trials in an attempt to determine the super-assembly structure by x-ray diffraction. Thus far no crystals have formed in our vapor diffusion trials, however, we are optimistic that they will form as precipitant concentrations in the trials equilibrate.

Evaluation of the Safety of Fish Consumption from the Lower Fox River. *TANYA CRUM (Richard J. Daley College, Chicago, IL 60652) Dr. David Miller (Argonne National Laboratory, Argonne, IL 60439).*

The safety of fish tissue consumption on the lower Fox River is unknown due to a lack of data. Detectable DDT and dieldrin sediment concentrations were used to estimate fish tissue concentrations based largely on the EqP approach and known BAF values. Safety of human consumption relative to these calculated values was also evaluated. It appears that the fish are safe to eat in terms of DDT and dieldrin concentrations in fish tissue. However, many factors can influence the reliability of these estimations casting doubt upon the findings.

CHEMISTRY

Theoretical Determination of Rate Constants for Volatile Organic Compounds + Hydroxyl Radical. *NICHOLAS SCAIEF (Washington State University) Dr. Bruce C. Garret (Pacific Northwest National Laboratory, Richland, WA, 99352)*

Radical reactions are very important to atmospheric chemistry, but are very difficult to study experimentally and theoretically. In principle, it is possible to determine rate constants for these reactions by *ab initio* methods. In the present work the reactions of some volatile organic compounds (VOC) with hydroxyl radical were examined. Minimum energy structures and ground state energies for the reactants, transition states, and products of reactions were found at various levels of theory including MP2/cc-pvdz and UCCSD(T) levels, using the Gaussian 98 electronic structure software package. DRDYGAUSS (Direct Dynamics with Gaussian) was used to trace out the minimum energy path along various reaction channels. Variational transition state theory (VTST) was used to obtain a rate constant from the topology of this energy surface. Changes in the level of theory used (selection of basis set and treatment of electron correlation) produce small changes in ground state energies and structures; the resulting potential energy surface becomes altered in the process. It was found that the theoretical rate constant depends exponentially on small variations in the potential energy surface topology. Thus, the level of theory has tremendous effect on the theoretically determined rate constant.

Ethanol Production from Rice-Straw Hydrolyzate Using *Zymomonas mobilis* in a Continuous Fluidized-Bed Reactor (FBR). *DARILYN DE JESUS (Polytechnic University of Puerto Rico, Hato Rey, Puerto Rico 00919) Dr. NHUAN P. NGHIEM (Oak Ridge National Laboratory, Oak Ridge, Tennesse, 37830).*

Rice-straw hydrolyzate obtained by the Arkenol's concentrated acid process was fermented to ethanol using a recombinant *Zymomonas mobilis* strain capable of utilizing both glucose and xylose in a continuous fluidized-bed reactor (FBR). The parameters studied included biocatalyst stability with and without antibiotic, feed composition, and retention time. Xylose utilization in the presence of tetracycline remained stable for at least 17 days. This was a significant improvement over the old strain, *Z. mobilis* CP4 (pZB5), which started to lose that capability after seven days. In the absence of tetracycline, xylose utilization rate started to decrease almost immediately. With tetracycline in the feed for the first six days, stability of xylose utilization was maintained for four days after the antibiotic was removed from the feed. In other words, the rate started to decrease on day 11. In the presence of tetracycline using the Arkenol's hydrolysate diluted to 48 g/L glucose and 13 g/L xylose at a retention time of 4.5 hours, 95% xylose conversion and complete glucose conversion were obtained. The ethanol concentration was 29 g/L, which gave a yield of 0.48 g/g sugar consumed or 94% theoretical. Using the Arkenol's hydrolysate diluted to 83 g/L glucose and 28 g/L xylose, 92% xylose conversion and complete glucose conversion were obtained. The ethanol concentration was 48 g/L, which gave a yield of 0.45 g/g sugar consumed or 88% of theoretical. Maximum productivity of 25.5 g/L-h was obtained at a retention time of 1.9 hours. In this case, 84% xylose conversion was obtained.

Ozonation of Produced Water from the Oil Industry. *MICHELE DINSMORE (Tennessee Technological University, Cookeville, TN 38505) Costas Tsouris (Chemical Technology Division at Oak Ridge National Laboratory, Oak Ridge, TN 37830).*

The oil industry, in the process of pumping oil from wells, generates "produced water," which is usually seawater contaminated with various organic substances. Before produced water is returned to the environment, it needs to be treated for the removal of the organics. One method to eliminate organic substances from produced water is oxidation, using ozone. Several experiments have been conducted in this study to instigate the effectiveness of ozone in oxidizing organic substances in real produced water from various oil companies. In these experiments, ozone was produced by a corona-discharge ozone generator and trapped in gas-tight bottles. Produced water was then injected in the bottles by a syringe at various volumes. The bottles were stored for an extended period of up to three days to make sure that the reaction was completed. After this period, the produced carbon dioxide from the oxidation reaction was measured, using a gas chromatograph. The total concentration of organics was also measured before and after the ozonation experiments, using extraction with poly-chloro-ethylene followed by infrared spectroscopy. Experiments were also conducted to investigate the effect of hydrogen peroxide on the oxidation process. Results show that ozonation is removing a substantial fraction of organics from produced water. The quantity of ozone needed for the completion of the reaction with a known quantity of produced water is also determined for the various sources of produced water. This information is needed in designing large-scale reactors for the treatment of produced water before it is recycled.

A Combinatorial Approach for Finding a Catalyst for the Direct Oxidation of Benzene to Phenol. *CHARLES HAMILTON (Texas A&M University, College Station, Tx 77840) Dr. Chris Marshall (Argonne National Laboratory, Argonne, Il 60439)*

A combinatorial method was developed for testing catalyst reactivity with hydrogen peroxide and benzene to form phenol at room temperature. To accomplish this, a 4-Aminoantipyrine assay process was developed to test for phenol at very low concentrations (500 ppb and above). This method involved doing 8 small scale reactions in microwell plates, doing a chloroform extraction in vial, and then performing the 4-Aminoantipyrine assay on the chloroform layer. This was done at least twice for each catalyst, and reproducibility is high. By this process, 50 catalysts have been tested, many in various conditions in a relatively short time span.

Rapid Analytical Technique to Identify Alpha Emitting Isotopes in Water, Air–Filters, Urine and Solid Matrices. *Nina Carte (University of Connecticut, Storrs 06269. Dr. Sal Scarpitta (Brookhaven National Laboratory, Upton, NY 11973).*

A Frisch Grid proportional ionization chamber was utilized at Brookhaven National Laboratory (BNL) to rapidly characterize and quantify a- emitting actinides in unprocessed water, soil, air-filter, urine and solid matrices. Instrument calibrations for the various matrices were performed by spiking samples with National Institute of Standards and Technology traceable (NIST) isotopes of Th-230, U-232, Pu-236 and Am-243. Detection efficiencies were typically 15-20% for solid matrices (soil, concrete, bricks, metal, etc.) and 45% for raw water samples. Instrument background over a 1200 channel a-energy range of 3-9 MeV is very low at 36 cph. At optimum operation, minimum detectable levels of 15 pCi g^{-1}, 0.2 pCi mL^{-1} and 0.4 pCi $filter^{-1}$ were achieved for 40 mg soil, <1.0 mL tap water (or urine) and 4.5 cm diameter filter samples, respectively, each counted for 60 min. Data and spectra will be presented showing the quality of results obtained using real samples obtained from the BNL Graphite Research Reactor. These BNL samples contained nCi to mCi amounts of actinides. The analytical advantages of this technique are: (1) minimal sample preparation is required, (2) no separation chemistry is involved and (3) no hazardous waste is generated. The benefits of this technique to the U.S. DOE are rapid turn-around-times (1-2 days in-house as opposed to off-site turn-around times of 2-3 weeks), and a cost savings of about $15,000 for the 30 samples analyzed so far for this project.

Synthesis and Characterization of SrPbO3 and Pb5B8O17. *Santiago Segarra (Turabo University, Caguas, Puerto Rico 00725) Dale L. Perry, (Lawrence Berkeley National Laboratory, Berkeley, California 00725).*

In recent years, people have had much concern with the state of their environment. The Scientific community feels pressed to develop new ways to detect lead and other heavy metals in the environment. One approach is the synthesis and characterization of model lead compounds such as Pb3O2Cl2. Using a solid state reaction has carried out syntheses like these. Pb3O2Cl2 has an orthorhombic-disphenoidal structure with an H-M Symbol (2 2 2) Space Group: P212121 X-Ray Diffraction: By Intensity (I/Io): 3.09(1) 2.78(0.7) 3.04(0.7) . Identification of the Pb3O2Cl2 was confirmed by the analysis of x-ray diffraction.

Investigation of the Amorphous to Crystalline Transition in Indium Tin Oxide. *Colleen Nehl (University of California, Santa Barbara, Santa Barbara, CA, 93107) David Ginley (National Renewable Energy Laboratory, Golden, Colorado 80401).*

Transparant conducting oxides (TCO's) are needed for applications like solar cells. These TCO's, may be able to be optimized by understanding the amorphous to crystalline transition in TCO's. We investigated this transition and the change in relevant electro-optical properties by using indium tin oxide (ITO) deposited at different temperatures and amounts of oxygen, and then annealing it to induce the change from amorphous to

crystalline. Our investigation revealed that resistivity usually decreases as crystallinity increases. We also saw slight increases in transparency with annealing. This research may offer new information about the crystallization mechanism for ITO, and possibly other TCOs. Understanding this amorphous to crystalline transition may, with further research, allow us to understand how to optimize electro-optical properties for current and future TCO applications.

Studying the Black Arts of Isolation and Crystallization of the Chromosome-Binding Protein MeCP2. *LAURA N. JOHNSON (St. Olaf College, Northfield, MN 55057), Gerard J. Bunick (Oak Ridge National Laboratory, Oak Ridge, TN 37830).*
MeCP2 is a chromosomal protein that plays a central role in gene silencing by binding to DNA containing the dinucleotide palindrome CpG (where p indicates the 5' phosphate group) which has been altered by the addition of a methyl group at the 5 carbon of the cytosine. MeCP2 then forms a complex with histone deacetylase, HDAC, a protein that condenses chromatin structure and contributes to gene silencing, and Sin3, a transcriptional repressor. MeCP2 is essential for normal embryonic development in the mouse, and mutations in the gene coding for MeCP2 are responsible for many cases of Rett syndrome, a sex-linked neurological disorder affecting human females. The structure of MeCP2 is of tremendous importance medically and to understand the underlying processes of transcriptional repression. The research reported here has resulted in the production of milligram quantities of protein and has identified preliminary growth conditions for the production of single crystals that will be used in solving the three-dimensional structure of MeCP2 by means of X-ray crystallography. This work involved expression of MeCP2 from prokaryotic systems and purification of the expressed protein by affinity chromatography. Screening precipitants as well as variations in pH, temperature, and salts identified solution conditions for nucleation and growth of pure protein crystals. Results from initial screens were used to design narrower or complementary searches until well- formed crystals were obtained. Isolation and crystallization of MeCP2 provides a means of correlating its structure with function, of comparing MeCP2 with other chromosome-binding proteins, and of discerning the structural association of DNA with other components of the chromatin assembly.

Hygroscopic Aerosols Roles in Atmospheric Chemistry **Presenter: Jed Atherley** *School Author Attends: Salt Lake Community College DOE National Laboratory Attended: Pacific Northwest Laboratory Mentor's Name: Stephen Joyce*
Hygroscopic aerosols play important roles in atmospheric chemistry. At specific humidity levels these aerosols can deliquescence, greatly altering size and reactivity. Hygroscopic aerosols undergo many changes during their atmospheric life times. Deliquescence and efflorescence can occur changing the morphology of the aerosol and cause fall out. To understand how these changes affect the atmosphere, scientific tools are needed to analyze these aerosols at microscopic levels. The environmental scanning electron microscope (ESEM) has the capability to simulate different humidity levels while the operator can monitor the morphology. NaCl, NaBr, and ammonium sulfate were used to test the ESEM and its abilities to create humidity levels accurately. Substrates were used to prevent unwanted nucleation on the surface of contact, which made for more consistent results. The deliquescence and efflorescence points where charted and compared to work previously done in this field. This showed us the accuracy and problems that may occur while using ESEM and provided direction for future work.

Investigation into the ion exchange properties of electroactive hexacyanoferrate film on a nickel substrate. *JOHN H. PARK (Sacramento City College, Sacramento, California, USA 95822-1386) Michael A. Lilga (Pacific Northwest National Laboratory, Richland, Washington 99355).*
In the process to recover lithium from brines, some lithium is lost because Li-K sulfate double salts precipitate over wide concentrations. Traditional ion exchange methods produce unacceptably high amounts of secondary waste and are not economically feasible for lithium purification. An electroactive nickel hexacyanoferrate film, which as a high selectivity for potassium over lithium, is being investigated as a means to perform a potassium/lithium ion exchange as part of a purification process. The film is deposited on a porous high surface area nickel electrode and ion uptake and elution are controlled by applying a cathodic or anodic potential, respectively. Alternately, the film has an affinity for K^+ over Li^+ and so the ion exchange between potassium and lithium is thermodynamically driven. Experiments were conducted with lithium uptake in water and methanol in efforts to maximize the life of the film. Temperature was fluctuated. Cyclic voltammetry was used to monitor the state of the film during experiments. Atomic absorption flame was used to analyze solution samples taken before, during, and after experiments. Results show the film can be used to extract potassium ions from solutions with high lithium ion concentrations.

Improving the performance and design of ion trap mass spectrometers. *Marino Morra (Salt Lake Community College, Salt Lake City, Utah) Michael Alexander (Pacific Northwest National Laboratory, Richland, Washington 99355).*
An ion trap is essentially an instrument that first stores ions and then facilitates their detection through mass-selective ejection according to the ion's mass/charge ratio. Important features of an ion trap mass spectrometer are the ability to retain ions for extended periods of time promoting ion-molecule chemistry, increase ion populations to aid measurements at low sample levels, and to perform multiple stages of mass analysis. Simion 3D version 6.0 is a very powerful PC based ion flight simulation program that models ion optics problems using 2D symmetrical and/or 3D asymmetrical electrostatic and/or magnetic potential arrays. This program was used to help in the development of new geometry, as well as refining RF and DC biasing schemes to optimize trap designs and performance for various applications prior to construction. A comparison of typical symmetric traps vs. the PNNL patented asymmetric trap was studied to find a more effective configuration.

Finding Fullerenes in Sedimentary Rocks *Author: Street, T. DOE Lab: Lawrence Berkeley Lab, Berkeley, CA.*
Commercial and naturally occurring fullerenes were isolated and studied with time of flight laser desorption mass spectrometry (LDMS). The fullerenes were studied to find a characteristic mass spectrum signature that could identify them as being extraterrestrial. Having an efficient technique for finding fullerenes and determining their origin would be an important advance in the study of extraterrestrial impacts on earth.

Kinetics of Reactions of Hydroxyalkyl Radicals with Thymidine, Thymine, and 1,3-Dimethyluracil. *ELIZABETH M. FRANZ and NICOLE M. STAIR (Whitman College) Dr. Jerome C. Birnbaum and Dr. James A. Franz (Energy and Health Sciences Division, Pacific Northwest)*
The free radical reactivity of the biologically important substituted thymines remains largely unknown for alkyl and ketyl radicals. To assess the fundamental reactivity of these substituted olefins, the kinetics of reaction of hydroxymethyl radical with thymidine, thymine and 1,3-dimethyluracil were determined by kinetic laserflash electron spin resonance spectroscopy (KESR). Hydroxymethyl radical was prepared by excimer laser photolysis at 308 nm of solutions of di-*tert*-butylperoxide and either thymidine, thymine, or 1,3-dimethyluracil in methanol as a function of temperature. The center ESR transition of the hydroxymethyl radical was monitored as a function of time following the laser pulse, for a series of experiments in which the concentration of the reacting olefin was varied over a temperature range of 253-323 K. Thymidine exhibited an Arrhenius rate expression for reaction with hydroxymethyl radical described by $\log(k/M^{-1} s^{-1})=(8.29\pm0.33)-(6.10\pm0.42)/q$, $q=2.303RT$ kcal/mol, errors are 2s. At room temperature, rate constants for reaction of hydroxymethyl radical were found to be 6.1×10^3 (1,3-dimethyluracil), 7.5×10^3 (thymine), and 6.9×10^3 $M^{-1} s^{-1}$ (thymidine). Attempts to observe the reaction of 2-hydroxyprop-2-yl radical with thymine and 1,3-dimethyluracil by KESR failed, consistent with very low rate constants (less than ca. 10 $M^{-1} s^{-1}$) for this radical. This is the first report of absolute rates of reaction of hydroxyalkyl radicals with this important category of olefinic substrates. The magnitudes of the rate constants for hydroxymethyl reactions are compared with other radical addition reactions. The observed reaction rates demonstrate that ribose-derived ketyl radicals will react very slowly, if at all, with uracil systems.

Methods in protein purification and crystallization for x-ray diffraction studies. *MARK HATOON (Richard J. Daley College, Chicago, Illinois) Andrzej Joachimiak (Argonne National Laboratory, Argonne, Illinois 60439).*
For a century scientists have used x-ray crystallography as a tool for gathering data on proteins and enzymes. Atomic structures have been solved and binding sights have been studied. Successful protocols for

purification and crystallization of proteins have been developed and utilized toward this end. Genes are engineered for nickel binding ability. This characteristic aids in selective purification. Purified proteins are then screened for ability and quality of crystallization using prepared chemical conditions. The advent and continuous improvement of x-ray sources worldwide guarantees the advance of structural biology. As a result, our understanding and appreciation of one of life's most beautiful and intriguing mystery's advances as well.

Lithium Ion Batteries. *MELINDA MAIER (Wingate University, Wingate, North Carolina 28174) Jong-Sung Hong (Argonne National Laboratory, Argonne IL 60439).*
The objective is to find the best possible Lithium-Ion battery. In the development of such a battery, there have been many different research ideas. Generated gases in the cell were analyzed. The cells are punctured and the generated gases are taken and run through a GC MS. Then the cells are centrifuged to get an electrolyte sample. Also the electrolyte sample is analyzed after the cell has been cycled and punctured. The analyzed data is then compared to data from a cell that has not been cycled. Comparisons on these cells were put into graph format so we could have a better understanding of what results were concluded. Conclusions were that we analyzed cells that were exactly the same and the results were that the gas generation was typically the same.

COMPUTER SCIENCE

Interactive Visualization in the CAVE. *MATTHEW AHRENS (University of Illinois, Champaign, IL 61820) Dr. Lori Freitag (Argonne National Laboratory, Argonne, IL 60439).*
The goal of this project is to design and implement an interactive tool for visualizing and interacting with numerical simulations in real time. To achieve this goal, sophisticated software tools such as the visualization toolkit (VTK) and the ALICE memory snooper (AMS) will be used to create a framework that allows scientists and engineers to access their data directly from the running simulation. A main focus of this project is to build a VTK visualization of data obtained from a memory application in 3-D environment such as the CAVE. The first step towards the completion of the goal of this project was to test the following: visualizing VTK data sets in the CAVE using only the information published by a server outside of the CAVE. The next major step in developing the application was creating a user interface. The main objective of the interface was to allow the user to manipulate the attributes of the data set, namely the isosurfaces, cutting planes, and vector glyphs. The control panel served very useful as an interface to the VTK object displayed in the CAVE. The result of the work on the application was the birth of AVIVA, standing for AMS VTK Immersive Visual Application. It is currently being tested on two different applications. The first is a data reduction tool on an octree data set designed by Dr. Freitag and Dr. Raymond Loy. The second is a PETSc application that solves for the flow around an M6 airwing.

Configuration Management (CM) of the Supervisory Control and Data Acquisition SCADA System for Power Management, using a new web-based CM database system on the Idaho National Engineering and Environmental (INEEL) Intranet. *Audra Wright (University of Idaho, Moscow, Idaho, USA), Mike Vaughn, INEEL (Idaho Falls, Idaho).*
Configuration Management is defined as a structured process for controlling the design requirements, documentation, and configuration of structures, systems, and components (SSC), all that are important to the protection of workers, the public, the environment, critical missions, and operations according the STD-107. Configuration Management helps maintain the balance between three very important relationships: design requirements, physical configuration, and the SSC documentation, by the design of its structured process. Maintaining this consistency among the design, configuration, and documentation provides many benefits for INEEL employees. The most important benefit is that the CM program provides us with the most updated information needed the make safe, sound, and timely decisions. The CM program also supports safe and cost effective operation and maintenance of INEEL facilities and equipment. It also provides a platform-independent method for employees from any location at the INEEL to access the most updated information to support SSC modifications. As you can see all of these benefits and more add to the importance of implementing the Configuration Management program site-wide.

Creating a Worldwide Meteorological Database. *ERIC WOODMAN (Community College of Southern Nevada, Pahrump, NV 89401) RAY GEORGE (National Renewable Energy Laboratory, Golden, CO 80401)*
A disparity exists in the quantity and quality of solar radiation and meteorological data that is available for other countries in comparison to the United States. The National Solar Radiation Data Base (NSRDB), an National Renewable Energy Laboratory project completed in 1992, provides hourly solar radiation and meteorological data from 239 locations over a period of 30 years in the United States. This is in sharp contrast to the data available globally. Current global data for horizontal solar radiation is available from the World Radiation Data Center for 1000 stations worldwide. NASA provides another source for monthly global horizontal solar radiation estimates. Some of the problems with these sources are the large distance between stations makes their data less reliable, and that the data contains no meteorological information for temperature, dew point, or wind speed (Marion, B). New Capabilities for Worldwide Weather Data Sets is a Director's Discretionary Research and Development (DDRD) project. The goal of this DDRD project is to address the inconsistency in global solar radiation and meteorological data available. According to scientist Ray George this DDRD will accomplish this by providing the capability to create modeled estimates of solar energy for any location and for any selected time. New Capabilities for Worldwide Weather Data Sets will facilitate the development of multi-year, hourly, global solar radiation and meteorological data sets and make them available on a DVD (digital versatile disk; formerly known as digital video disk) format. The DVD-R will provide a significant advantage in both size and accessibility over the current tape format used, and because of the wide adoption of the DVD format these sets will be highly portable.

Long-Term Stewardship Needs and Technology Baseline 2000 Website Development. *STEPHANIE HALLOCK (University of Idaho) Cathy Plowman (Idaho National Engineering and Environmental Laboratory, Idaho Falls, Idaho 83415)*
Long-Term Stewardship is an important concept that is beginning to emerge into the public mindset. An inventory of technologies and the needs associated with various DOE sites was done in order to get an understanding of what lies ahead in the integration of Long-Term Stewardship into the DOE. A website was created to display the information gathered in a way that can be accessed by personnel at various DOE locations as well as the general public. The website was first developed using static web pages, a process that was time consuming and inefficient. Later revision of the web page resulted in the use of Cold Fusion software to turn the website into a dynamic system of less then 10 pages. Cold Fusion combines HTML and information from a database to create a web page. Using this software also allowed for the development of better graphics and page layout. It is hoped that this website will be a useful tool for those who are directly involved with Long-Term Stewardship.

Porting the Visualization Routines of PETSc into Win32. *CHAD CARROLL (Lake Forest College, Lake Forest IL 60045) Satish Balay (Argonne National Laboratory, Argonne IL 60439)*
PETSc, the Portable, Extensible Toolkit for Scientific computation, is a suite of routines and data structures that provide scalable solutions for scientific applications that are modeled from partial differential equations. PETSc is still being developed and currently is ported to most Unix platforms as well as Microsoft Windows (Win32). However not all features of PETSc are available on Win32. Specifically the visualization functionality was lacking on Win32. In order for the graphical functions of PETSc to work on a Win32 machine (Windows NT or Windows 2000) all Unix native graphical routines of PETSc need to be ported into Win32 code. Once these routines for Win32 are in place programmers on Win32 machines will be able to use the complete functionality of PETSc. Because of some of the fundamental differences in the system operation of Win32 compared to that of Unix this project became much more than a simple Win32 coding problem. The reason behind the difficulties is due to the fact that in order for the PETSc backbone to use this new code all function calls and routines need to be in the exact format of the Unix code. My personal contribution to this porting project has been in the graphic visualization functions.

Information Management Approach to the Virtual Human. *JOY E. WRIGHT (Christian Brothers University) of Dr. Richard Ward and Kara Kruse (Computational Physics and Engineering Division at Oak*

Ridge National Laboratory Oak Ridge, Tennessee 37831-6064)
The Virtual Human Project has the vision of structuring the complete human body with working organs and body functions to appear on computers to aid in medical diagnosis. Towards this goal, researchers at ORNL have developed a Java client/server architecture for linking physiological models written in various programming languages. This architecture takes advantage of Java Remote Method Invocation (RMI) to connect a Java client-user interface to servers where the physiological simulation codes reside. Forms for describing the models were created using XML (Extensible Markup Language) documents to describe the model variables, parameters and initial conditions for each model. A DTD (Data Type Definition) file was used to control the information being entered on the web-based forms that were created using Java applets. The information was retrieved and stored in a database using JDBC (Java Database Connectivity). The forms are needed to assist the users of the various models in entering the appropriate information to start the different simulations. They will also help keep control of administration's accessibility to change relevant data structure and default values to the models. The main purpose of using XML and DTD in creating forms is to provide a very flexible, modular, distributed environment where the model, model data, and user interface are separated. Such an environment allows the rapid modification of current models and integration of new models into the environment.

Software Development for the Intelligent Monitoring System for Safeguards Applications. *CORTEZ L. HARVEY JR. (Harry S. Truman College / DeVry University) Kirsten Laurin-Kovitz (Argonne National Laboratory, Argonne IL 60439)*
Nuclear material is stored throughout the world and monitoring the material is a big job. In 1996, the International Atomic Energy Agency handled over 1 million data records as part of its nuclear material monitoring activities. Creating software systems to assist with nuclear material monitoring can improve the process. In the Intelligent Monitoring for Safeguards Applications Project, we are developing these software systems. In developing the software, we have three main goals. We need software that can monitor nuclear material, so that the process will be more efficient. We also want the safest possible situation when it comes to nuclear material, so we need software that improves safety and we need to protect ourselves and the material from being tampered with, so the safeguards system is specifically designed to enhance security. We can save money by creating these systems because we will not need as many people to work in these areas. In addition, being able to monitor this material over the Internet would be a great advantage. Two software programs were developed which providing different ways to view the data from nuclear material sensors. The first program is a program that graphs nuclear data in real time. The second program averages out data from over different times and puts them in a table.

Automation of the 0.8-m Telescope at Rattlesnake Mountain Observatory. *CULLEN ANDREWS (Eastern Washington University) Ken Swanson (Environmental and Health Sciences Division, Pacific Northwest National Laboratory)*
The Rattlesnake Mountain Observatory is on a remote hilltop in the Columbia Basin of Washington State. Work is being done to automate the 0.8-m reflecting telescope there and make it accessible through the Internet. Local high schools will use it for education. We used video streaming to give a live presentation of sunspots on the lab's intranet. We designed a flat field screen for our CCD camera to correct variations in pixel sensitivity. Taking an image of a uniformly bright surface and dividing the raw CCD frames does this. Our flat field method is a piece of foam board inside the dome, which is illuminated by two adjustable lamps with large diffusion screens. The CCD camera has not functioned during testing. Emulsion photography through the telescope consumes more time than is practical, and it is impossible for dim objects because of tracking errors. There is now software to adjust the tracking rate, but having the computer adjust it by reading encoders may be the best option. The dome is being renovated so that the computer controls it. All of the observatory's functions must be computer controlled for full automation. This is still sometime away, but it is much closer now than in June. We can now find objects by looking at encoder readings instead of hunting with a guide scope. This makes the telescope many times more efficient. Some more work and modern equipment will unlock the observatory's great potential.

Automated Security Scan. *M. PECKFNL, Yershov (Argonne National Laboratory, Argonne, Illinois 60439).*
Every organization should seek consultation from recognized security experts who know how to integrate and implement security solutions. These experts should be highly trained and certified by the security product manufacturers. Their reputation should be undisputed by security manufacturers, major carriers, Internet Service Providers, government agencies, and corporations both large and small. Efforts need to taken to ensure your network is free from outside interests, (hackers) who would otherwise make your network their own playground. These individuals will stop at nothing until they have your system compromised and all your personal files are either deleted, or they can get into your system to just play around with your files. There are many ways to circumvent these hackers and to ensure that your network, and everything that travels across it are secure. One way I learned is to use ISS (Internet Security Systems) , they have a full array of scanning devices that can thwart any penetration by these people. In setting up your system's defenses, you first need to have your network specialist configure your network to lock out any intruders from the network side of things. Firewalls need to be set up properly and all other security aspects need to be up to speed. Then comes the ISS installation, once you have it installed you can run a scan on your own computer or others, provided you have their permission. The variables can be set up to fit your company's individual needs. The scan will check all of your vulnerabilities and generate a report based on those findings.

Phase I of Infrastructure Review, Standardization of UPS Systems and Generator Systems in PASSPORT. *Anthony S. Denniston (Idaho State University, Pocatello, Idaho 83204) Dudley Russell and Kevin Brown (INEEL, Idaho Falls, Idaho 83415).*
Quality and reliability are directly related to the maintenance of equipment, such as with UPS and Generator. Investigating the maintenance of these two types of standby power systems was done in several steps. The major steps were to identify the level of each individual system, identify the frequency of the maintenance, in accordance with NFPA 110 and NFPA 111, and verify visually and gather more information about the standby power supply systems to improve the maintenance database. The next major step to identify the systems was found in the maintenance management program, PASSPORT. Then to generate a standard work order, which contained the different tasks needed to generate the work orders at different frequencies for the standby power supply systems. The final task was to input the model work orders to be used for performing the different maintenance. The effective maintenance of standby power supply systems will improve the quality and reliability of the systems.

Automounting and Resources Sharing with Linux, SunOS and Open BSD. *MARIA DEL MAR ALVAREZ ROHENA (University of Puerto Rico-Bayamón Campus, Bayamón, Puerto Rico 00959) EVERETT HARVEY (Lawrence Berkeley National Laboratory, Berkeley, California 94720).*
When a computer network is composed of hundreds of computers it is important to keep most of the computers sharing a common set of resources to avoid moving from one computer to another searching for programs needed. In Unix-based systems using the Yellow Pages and automounting tools like the Amd Automount Daemon and Autofs can do this. With Yellow Pages, Unix computers can share resources, such as user passwords, and with automount all the users sharing the user passwords can see their same directories in any Unix computer. An OpenBSD computer was configured as a YP Master Server and NFS server. One Linux computer was set as a YP Client binding to this computer and another one was set as a YP Slave Server of the OpenBSD computer. The Linux computer that was set as a YP Slave was configured to automount using autofs from a Sun computer and using amd from the OpenBSD computer. By doing this, many common resources were shared between OpenBSD, Linux and SunOS computers.

Integration of File Transfer Protocol into the Distributed-Parallel Storage System. *MICHAEL STOOPS (Washington State University, Pullman, Washington 99163) BRIAN L. TIERNEY (E. O. Lawrence Berkeley National Laboratory, Berkeley, California 94704)*
The Distributed-Parallel Storage System (DPSS) is a parallel, super-

striped, distributed storage system. DPSS installations serve scientists worldwide by providing high- speed storage for large data sets. As the DPSS project currently stands, its product does not serve any common interface. That is, one must write a custom program to make use of a DPSS installation. The solution to this problem is to integrate File Transfer Protocol (FTP) service into the DPSS Application Programming Interface (API). With integrated FTP, users may use DPSS with common client programs such as Netscape Navigator and Microsoft Internet Explorer. The Globus Group's Grid Security Infrastructure FTP (GSI-FTP) FTP extensions were selected to provide necessary security support. A proof-of-concept FTP server shows FTP can be used to interface with a DPSS.

Upgrading a Database for Structural Testing. *RICARDO SANTILLANO (Dona Ana Branch Community College Las Cruces, NM. USA 88021). ARLINDA HUSKEY (National Renewable Energy Laboratory, Golden, CO 80401)*
Upgrading a Database for Structural Testing using a barcode system would save time and money. (National Renewable Energy Laboratory) NREL's structural test facility is primarily used for structural testing of full-scale wind turbine blades for NREL's subcontractors and wind industry partners. The turbine blades are tested by the use of several instruments that need to be calibrated. There are two types of testing that are accredited fatigue testing and static testing. Because they are accredited test, they must meet the requirements of ISO Guide 25. All of the instruments are stored in the database with the history of the instrument including the date of calibration, Location of instrument, the calibration due date, and comments about the instrument. A barcode system using a portable data collector called the Falcon 310 would best fit the needs for the database.

Solar Data Quality for Climate Change Research. *PAUL (FILEMON) RAEL (Pueblo Community College, CO 81006) MARY ANDERBERG (National Renewable Energy Laboratory, Golden, CO 80401)*
Understanding exactly what affect solar energy exchange has on the Earth- ocean-atmosphere system is important to understanding the system as a whole. To further our knowledge of this energy exchange, the Atmospheric Radiation Measurement Program has implemented three data acquisition sites in climatically diverse areas to record the six constituents of solar energy reaching the atmosphere throughout the year. This data will be input into existing models to further ARM's comprehension of atmospheric mechanics and climate change. The data collection process is not perfect, however, and this fact renders a mandatory quality control apparatus known by the acronym, SERI QC in this case. SERI QC is a battery of tests that are designed specifically for terrestrial solar energy data quality assessment. In the case of the data described in this paper- the1999 ARM data for the Southern Great Plains site in Kansas and Oklahoma, SERI- QC deemed 85.2% of all possible daytime data accurate to 95% or better. This figure tells us that while data quality is relatively high, there is plenty of room for improvement.

Sounding Healthy: The Virtual Human's Need for Speed; Parallelizing Computational Fluid Dynamics Code. *Todd L. Miller (Haverford College, Haverford, PA) Kara L. Kruse (Oak Ridge National Laboratory, Oak Ridge, TN) Dr. Richard C. Ward (Oak Ridge National Laboratory, Oak Ridge, TN)*
The Virtual Human project connects three-dimensional anatomical and dynamic physiological models of the human body to investigate a wide range of biological and physical responses to various stimuli. As part of the Virtual Human project, computational fluid dynamics — numerical approximations of the response of fluids to forces — is used to model generation of lung sounds. Lung sounds in the middle airways of healthy people are produced primarily by complex vortex flow due to the multiple curved branchings of the airways. Because of the accurate data, complex geometry, and requirement for fine details in the fluid flow, the current simulation code ('PHI3D', developed at Oak Ridge National Laboratory by Dr. Paul T. Williams) runs unacceptably slowly. The parallelization of the finite-element basis matrix formulation used custom-developed codes and MPI, and succeeded in reducing run time approximately one-third in the best case. Replacing the matrix equation solvers with the PETSc parallel package (developed by Argonne National Laboratory) unexpectedly caused the code to run twelve times slower . Explanations and future directions are detailed.

Web-Based Application Development for Recording Staff Activities. *Kristopher Daley (University of Tulsa, Tulsa, Oklahoma 74104) Michael J. Sale (Oak Ridge National Laboratory, Oak Ridge, TN).*
Every year the Environmental Sciences Division of ORNL must complete a form known as the "Yellow Sheet." This form serves as the record of all events in which an employee participates in during a fiscal year. The current format of the "Yellow Sheet" involves the employee writing down all their information, passing it to the secretary, the secretary typing it in, and then submission. This process is very slow and redundant, hence the need for a better system. The solution is to design a database to hold the employees' information, while adding a web interface for ease of use. The web interface will allow all users to enter their information by themselves from anywhere, when events happen. This is a substantial improvement over the old system because you can enter information in real time, rather than trying to remember everything all at once at the end of the fiscal year. This saves time, increases productivity, and allows less chance of error as opposed to the old system. The new system incorporates a database designed in Microsoft Access 2000 and a web interface programmed in ASP. This new web interface also incorporates a searching feature that will allow users and supervisors to see their information in any interval, be it a week, a month, a year, or 5 years. The new system will benefit the department by providing an efficient and effective way of reporting their activities for performance evaluations.

Integration of the Left Heart Model into the Virtual Human Interface. *DAÑON PRICE (Emory University, Atlanta, GA 30322) Richard Ward (Oak Ridge National Laboratory, Oak Ridge, TN 37831)*
The Virtual Human Interface is a visualization tool that combines computational models and data about the human body into one virtual model for simulation, study, and implementation of various other applications. The interface integrates computational models of human organs as a means to study their function and operation individually and interactively. One type of model emulates the operation of physiological systems using electronic components combined into fully functional electronic circuits that having Kirchoff's laws applied, produce ordinary differential equations. These differential equations, after undergoing a numerical integration technique, subsequently produce graphs for monitoring the effects of the modifiable parameters. One such computational model created by Vincent C. Rideout (Mathematical and Computer Modeling of Physiological Systems, Prentice Hall, 1991) is the circuit equivalent for the left heart, LH-PF-3. LH-PF-3 is the third of a series of left heart models that demonstrate gradual improvements in circuit design and mathematical implementation to ultimately develop an anatomically correct and complete cardiovascular loop. A configuration file was created implementing the eXtensible Markup Language (XML) controls construction of this model. Integration of this and other models serves as a means of universalizing the complete interface for future additions of models of the heart and other human organs.

Evaluation and Application of Techniques Used to Create and Maintain a Viable and Useful Web Page. *Amber Sallerson (University of Maryland, Baltimore County, Baltimore, Maryland 21250) Dr. Ruth Ann Manning (Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830).*
The creation and maintenance of web pages has become a major concern in all facets of industry and personal use. The creation of a web page, while perhaps elementary in thought, introduces a plethora of choices to the creator. The ultimate goal of the designer is to construct a page that is functional and flexible, interactive and maintainable, informative, and creative. Central decisions as to the choice of server and platform are made on an individual basis according to the specific needs of the informant and the information that is to be presented. The HTML language was the main language utilized on the Unix platform to create the Research Alliance for Minorities (RAM) web page. A regular web based server was chosen over that of a client server and the requested information was organized in such a manner as to provide a logical and useful path of information. Techniques were chosen based on observations of similar applications, familiarity with such techniques, and technique capabilities. The resulting web page will be posted by Oak Ridge National Laboratory and will be available for public viewing and divisional maintenance.

Map Networking. *MARIO TOBIAS (University of Texas at Brownsville, Brownsville TX 78526) and Keith Sanford (Oak Ridge National Labora-*

tory, Oak Ridge, TN 37831-6069).
Networking, the interconnection of computers that work on the same domain and are able to share information, is an essential part of all big industries and companies all over the world. Networks are formed using several components; Bridges, Switches, Hubs, Routers, etc. Network maps exist to have a specific and very accurate location of these devices. Maps were created to describe all the connections of each port, of each bridge located at Y-12. All the locations, that have components of the network, were visited. Visio 2000, a software program designed for the construction of Network Maps, will be used in order to interpret the connections of each location. This project will give the CIND division a very detailed overview of all the bridges at Y-12.

Moving Files or Folders Between Web Servers Across the Internet Utilizing HTTP. *Francisco (Frank) Concha (Big Bend Conimunity College, Moses Lake, WA. 98837) W. Boyd Taylor (Pacific Northwest National Laboratory, Richland, Washington 99355).*
The Internet has become the mainstream choice of businesses for the gathering and manipulation of data. The processes for moving data over the Internet have long been available to the general public. Scrutiny of such data has been maligned by would be hackers utilizing methodology to circumvent traditional processes. File movement between separate sites on the World Wide Web has been a security issue and will continue to be so until applications written specific to end users is developed in house. Therefore, in an attempt to determine the feasibility for a method that will be user friendly, and secure has been examined. My following documentation will explore the utilization of external components already in place by public users and the utilization of the component(s) in addition to programs driving the test. It will be determined if it is at all possible to move a file across H-TTP rather than using a public accessible application like FTP. Once this specific project milestone is accomplished, an additional phase will be created whereby, additional processes of file movement will take place, to include: moving a file from a host server to a remote server, moving all files of a unique folder to the remote server, moving all files and folders within a unique tree to remote server, utilizing a comparison algorithm to test file and file structure maps whereby host server will be updated utilizing standard file management utilities to delete, create, or update files or folder or combinations there of.

Computer Programming. *KRISTI DRAGOO (University of Washington, Seattle, Washington 98195). Laura MS Curtis (Battelle Pacific Northwest National Laboratory, Richland, Washington 99355).*
During my internship at Battelle Pacific Northwest National Laboratories, I learned how to write Perl, a commonly used programming language. I wrote programs that will be additions to the projects my mentor is currently working on. The largest project this summer was a program for the Topic Islands project. Topic Islands is a visualization system prototype designed to scan through a document and generate a rough outline. In order to run a document through Topic Islands, certain directories and files must be made specifically for that document. Instead of having customers do this by hand for each document they wish to run on Topic Islands, they had me create a program that would do this. The program I created is titled corpora.pl. By running the document through corpora.pl first, all of the necessary directories and files will be made to successfully run Topic Islands on that specific document. This will assist the users of Topic Islands and make the product easier to use.

Intelligent Agent Technology in Remote Sensing. *SAM REID (University of Colorado, Boulder, USA 80309) Brian D. Moon (Pacific Northwest National Laboratory, Richland, Washington 99355).*
Remote sensing data processing is computationally expensive and no algorithms have been developed which are both automated and suited to varied data sets. Project ARCA (Advanced Registration and Calibration techniques using software Agents) is developing an Agent-based processing environment for remotely sensed data. Software tools to transmit, parse and act on KQML performatives have been coded and tests with fundamental image processing functions and image registration have proved successful. An Agent oriented solution offers the ability to process data in dynamic processing fields in which the tools available to a given Agent may change with time, and dynamic problem domains in which the data to be processed require different paths of processing. Further advantages offered by an Agent-based solution include: a shared computational load conferring increased speed of execution, robustness against hardware malfunction of any computational element and the ability to exchange information and processing abilities with other populations of Agents.

Colonie Site Remediation Project. *ROBERT T. JOSLIN (Richard J Daley College) David Miller, Ph.D. (Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Il 60439-4845)*
My assignment at the EAD was to evaluate, assess, and make recommendations, if any, and make changes to the Colonie Remediation Public and Professional Web Sites. The first thing that had to be accomplished was to research and familiarize myself with the research materials of the project and get a better understanding of a remediation project. Therefore, I could understand the data in the web site and how it was organized.
Then, I had to accomplish the task to build an assortment of demonstrator web pages of the entire web site so the director had several alternatives on how he would want to proceed with the reconstruction of the web site.

Development of the Materials Science Web Page. *DAVID LEHMAN (University of Wisconsin, Madison, Wisconsin 53705) JACKIE JOHNSON (Argonne National Laboratory, Argonne 60439*
The World Wide Web has become an integral part of the lives of many people across the globe. It is becoming more and more important for organizations to have a functioning Web site. Such a Web site allows people to obtain information about the organization quickly and easily from anywhere. The Materials Science Department at Argonne National Laboratory has been running a Web site for several years and has not fully updated it for the last four years. The Web site needed to have a new design applied to it as well as updating its content.

Installation and upgrade of software, new printer configuration and migration from an old application server to a new application server using Windows operating systems. *Jolly M. Pazhai (Truman College, 1445 W. Wilson Avenue, Chicago, IL 60640.) William McDowell (Argonne National Laboratory, Argonne, IL 60439-48456)*
Migration from the old application server called APSNT3 to the new application server called LEAD was done to provide more storage and to provide faster access to users using this server. Installing new software allowed automation of many tasks that were otherwise manual and very time consuming. Upgrading software enabled the users to access the latest technology for improved performance. Configuring printers to the new servers SODIUM and LEAD resulted in more unified central administration. Disconnecting File and Print sharing option improved network security. After completion of this project, the network administrators will be able to control, maintain, and administer the network in the Advanced Photon Source in a timely, efficient manner.

ENGINEERING

Optimization of Electric Power Systems for Off-Grid Domestic Applications: An Argument for Wind/Photovoltaic Hybrids. *Jennings, Wendy (Colorado State University) and Jim Green (National Renewable Energy Laboratory)*
The purpose of this research was to determine the optimal configuration of power sources relevant to different regions in the United States. The hypothesis was that regardless of region, the optimal system would be a hybrid incorporating wind technology, versus a photovoltaic hybrid system without the use of wind technology. The method used in this research was HOMER, the Hybrid Optimization Model for Electric Renewables. HOMER is a computer program that optimizes electrical configurations under user defined circumstances. According to HOMER, the optimal system for the four regions studied (Kansas, Massachusetts, Oregon, and Arizona) was a hybrid incorporating wind technology. The cost differences between these regions, however, were dependent upon region. Future studies will be necessary as it is difficult to estimate meteorological trends for other regions.

Reconstruction of Pore Networks from Analyses of Imaged Slices of Porous Materials for use in Two-Phase Flow Simulations. *Brandon M. Peden (Western Washington University, Bellingham, Washington 98225). Liviu Tomutsa (Lawrence Berkeley National Laboratory, Berkeley, California 94704).*
The oil industry is interested in an efficient and accurate way of modeling pore structures in oil reservoir rock and simulating fluid flow in these structures in order to determine methods of increasing oil recovery.

Current techniques are time-consuming, limited in scope, or not rigorous. Instead of using these techniques, researchers at LBNL are synthesizing rock structures from grain-size statistics of real rock (depositional model), analyzing images of this synthetic rock to create an approximate pore network, and running flow simulations on this network to determine the important fluid flow parameters necessary for determination of proper methods of oil recovery. The image analysis portion of this process is accomplished with the use of 3DMA, developed by W. Brent Lindquist at SUNY. There are four steps in the image analysis of depositional models: medial axis generation, modification of this medial axis, throat extraction, and pore network output. Using three different models, one regular hexagonal close packed (HCP) model and two irregular depositional models, we carried out the four steps. After the pore network outputs were generated, studies were done on the accuracy of these networks. The HCP network was run through ANetSim, developed by Tad Patzek of LBNL, to run flow simulations. The results of the flow simulations were good for the HCP model. Inspection of the different image analysis steps in 3DMA indicated that the medial axis algorithms were robust, but some of the routines in medial axis modification and throat extraction yielded non-physical results.

Alternative Transportation Technologies: An Experience with FutureTruck 2000 Competition. *GREGG GRUEN (Illinois Institute of Technology, Chicago, Illinois 60616) Robert Larsen (Argonne National Laboratory, Argonne, IL 60439)*
Out of all the automobiles being sold today, a large number are sport-utility vehicles. Sport-utility vehicles are typically larger than ordinary vehicles and consumer a larger portion of gasoline. To combat the gasoline and emissions problems that these vehicles bring forth, new technologies need to be developed to find alternative, cost effective sources of energy. Argonne National Laboratory has partnered with General Motors and the US Department of Energy to allow a group of university engineering student to attempt to use hybrid electric technology to improve the fuel efficiency of a sport-utility vehicle. Argonne organizers work year-round with sponsors and teams preparing one of the country's premier engineering competitions. FutureTruck 2000 was an overall success, proving the feasibility of this new technology in a sport-utility application.

Palo Alto Heritage Center Energy Savings Analysis, *BRAD M. AVERY (Colorado State University, Fort Collins, CO 80523) DR. ANDY WALKER (Federal Energy Management Program, National Renewable Energy Laboratory, Golden, CO 80401).*
The Palo Alto Heritage Center will be built near Brownsville Texas to commemorate the first battle of the U.S.-Mexican War. Due to several acts, initiatives, and Executive Orders, energy efficient design was a concern for this project. The Energy-10 software program was the primary tool used in the analysis. Energy-10 conducts an hour-by-hour annual analysis of twelve strategies to apply to a reference case building to generate a low-energy case building. Daylighting, glazing, shading, energy efficient lighting, insulation, air leakage, high efficiency HVAC, and HVAC control strategies were considered for this project. Specific roof and wall window modifications and wall construction modifications were also analyzed with Energy-10. Photovoltaic systems and natural ventilation are beyond the scope of Energy-10 and were analyzed separately. Results indicate that daylighting and high efficiency HVAC strategies offer the greatest annual energy cost savings, with both strategies saving about $2,000. With all energy efficient strategies and building modifications considered together, the low-energy building generated recognizes a 43% annual energy use savings over the reference case building with no energy saving strategies applied.

Energy Efficient Fixtures for Real World Applications, *Laura Schloss (Gonzaga University, Spokane, WA 99258) Michael Siminovitch and Jeffrey Mitchell (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*
Improving energy efficient light fixtures is the primary goal of the Energy Efficient Lighting Laboratory. Various photometric techniques are implemented as a crucial element for the designing of energy efficient lighting technology. Currently, instruments such as a Gonio-Photometer and an Integrating Sphere are used for testing fixtures and bare lamps. A Downlight Integrating Chamber was built at minimal cost and will ultimately be capable of testing downlight fixtures for a greater variety of applications than current methods being used. Fixture controls are another important element of saving energy. A modified occupancy sensor was installed on the lighting system of a beverage machine which dims the machine's lights when no one is around. This Energy Smart technology saves energy without compromising the marketing technique of beverage machine companies. Using the energy efficient technology described herein will benefit the E.P.A. regulatory system, improve production for lighting manufacturers, improve marketing for beverage machine companies, and save millions of dollars in energy consumption.

Digital Inverse Modeling of Multiphase Flow Through Porous Medium. *Robert Reichenbach (Hope College, Holland, Michigan 49423) Liviu Tomutsa, Stefan Finsterle (Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, California 94720).*
Increased efficiency of oil reservoir drilling, in addition to being a concern of the Department of Energy, is a very important topic for oil companies. Since modern technology allows for only 30 percent of an oil reservoir to be utilized, further development of technology would be very beneficial from both an industry and environmental standpoint. Because few pieces of the puzzle of reservoir flow dynamics can be observed, the only way to practically understand the reservoir flow is through computer simulations. We are developing a microscopic level pore network simulation that will use simple data inputs of grain sizes to effectively model core plug simulations. Part of creating an accurate program is having correct input data. Two styles of grain size distributions were measured in which ground up grain was deemed more accurate than a thin section distribution. To determine if the pore network simulation is accurate, a current, well accepted macroscopic computer simulation known as iTOUGH2 was used to determine rock characteristics that could be compared with the pore network simulation.

Improving the performance and design of ion trap mass spectrometers. *Marino Morra (Salt Lake Community College, Salt Lake City, Utah) Michael Alexander (Pacific Northwest National Laboratory, Richland, Washington 99355).*
An ion trap is essentially an instrument that first stores ions and then facilitates their detection through mass-selective ejection according to the ion's mass/charge ratio. Important features of an ion trap mass spectrometer are the ability to retain ions for extended periods of time promoting ion-molecule chemistry, increase ion populations to aid measurements at low sample levels, and to perform multiple stages of mass analysis. Simion 3D version 6.0 is a very powerful PC based ion flight simulation program that models ion optics problems using 2D symmetrical and/or 3D asymmetrical electrostatic and/or magnetic potential arrays. This program was used to help in the development of new geometry, as well as refining RF and DC biasing schemes to optimize trap designs and performance for various applications prior to construction. A comparison of typical symmetric traps vs. the PNNL patented asymmetric trap was studied to find a more effective configuration.

Drafting and Engineering. *Amanda Benally (Mesa Community College, Mesa, Arizona, 85202) Jeffery P. Pittman (Pacific Northwest National Laboratory, Richland, Washington 99355).*
Since the beginning of civilization, engineering has been a way of making our everyday lives easier. Through engineering we've created technology. Technology has linked us to a means of better communication. When dealing with the engineering process, it is crucial that the right information is being exchanged. The saying, "a picture is worth a thousand words," still holds true. Drafting is a method used to express what a person has in mind in terms of construction for the actual project or product. As the years have gone by, technology has become more complex then in previous years and will continue to do so in the years to come. Society will always co-exist with technology therefore as long as we exist we will need to improve the way we communicate. AutoCAD is a way we have been able to create plans on computer. AutoCAD is used to create myriad images for every drafting and design. Its is software used for architecture, engineering and mechanical work. AutoCAD has been the platform for communication among engineers for years.

Characteristic curves of Quantum Cascade Lasers Using a LabVIEW Controlled Source. *ALEX BRADLEY (Washington State University, Pullman, Washington) David Sheen (Pacific Northwest National Laboratory, Richland, Washington, 99352).*
The Quantum Cascade Laser is a fairly new development in the laser industry. The Infrared Systems Development group at PNNL uses the QCL in various experiments. Bell Labs, who manufactures the QCL,

does not have the time required to evaluate and characterize every unit they produce. Computer programs were needed to produce characteristic curves of the QCLs using a programmable source unit. Two LabVIEW programs were developed to control Keithley model 238 source/measure units. One of the programs produces a current vs. voltage curve of the QCL and the other uses an optical power detector to produce an optical power vs. current curve. An instruction manual for operation of the programs is included in this paper.

Material Characterization Using the V(z) and Resonance Techniques in Acoustic Microscopy. *RANDALL FIELDING (University of Idaho) Dr. Morris Good (Pacific Northwest National Laboratory, Richland, Washington 99352).*
The resonance and V(z) materials characterization techniques of acoustic microscopy are both used in industry currently. However, neither of these two techniques are currently in use at the Pacific Northwest National Laboratory. This research was performed in order to build a foundation whereupon a program utilizing these two characterization techniques can be developed. The V(z) experiments were carried out using a ten cycle tone burst, a homemade transducer, and a Sonix Flex Scan-C acoustic microscope system. Measurements were taken on Pyrex, tungsten, and brass samples. From these measurements the surface wave velocity of the materials was calculated, to within 10% of the actual value. The surface wave velocity can then be used to calculate other material characteristics. For the resonance work, the same Sonix system was used except with a tone burst to map out changes in thickness of a test piece machined from a polycarbonate plastic. Standard B-scan data from the test piece was digitized and converted into a power spectrum. As the thickness changed so did the power spectrum. The power spectrums were then plotted against position and frequency and amplitude was represented as color. As the thickness changed the position of the minimums and maximums in the power spectrum also changed. By observing these changes over an area the changes could be mapped out.

ENVIRONMENTAL SCIENCE

Research on the Kyoto Protocol for limiting the regulating the emission of Carbon dioxide into the environment. *ROSALINDA RAMOS {South Texas Community College, McAllen, TX, USA 78501} Gale Boyd, Ph.D. Economist {Argonne National Laboratory, Argonne, Illinois 60439}*
The Kyoto Protocol stimulates countries to find solutions to improve the environment by targeting the greatest contributor to the destruction of the atmosphere and environment, carbon dioxide (CO_2). Carbon dioxide molecules causes the temperature of the earth's atmosphere to rise, thus, causing various harms to the earth's climate. If global warming is not controlled it could lead to the depletion of the environment. Dramatic changes in weather and temperature are great examples of the spill down effect that causes the decline of such things as the coral reefs, the polar ice cap and causing damage related to changes in weather patterns, affecting the poorest countries which are densely populated and unprotected. The Kyoto Protocol encourages developed countries and developing countries to band together and slow down global warming. It provides several options to regulate the emissions of carbon dioxide such as tradable credits, Joint Implementation (JI), or the Clean Development Mechanism (CDM). Passing the protocol will have lasting effects on the economies of all the countries.

A Possible Mechanism for Lignin Model Synthesis. *Cheryl Loveless (University of Portland, Portland, Oregon 97203) Joe Bozell (National Renewable Energy Laboratory, Golden, Colorado 80401).*
Lignin is a potentially valuable renewable resource. Making up 30% of the dry weight of wood, it is the second most abundant organic matter on the Earth. Lignin is considered a by-product of wood pulping. Because of its complex structure, lignin is difficult to turn into other usable products. Thus, the production of accurate and usable lignin models is important in renewable chemistry. Performing reactions on lignin is impractical. A similar reaction may be performed on a lignin model, the results of which can be easy to interpret. The better the lignin model, the more likely reactions using the model will apply to lignin. A new method of synthesizing lignin models using orthoesters has been investigated at the National Renewable Energy Laboratory. The method reacts orthoesters with phenols to produce a biphenyl lignin model. This method produces two products, only one of which is the desired lignin model. The mechanism of this synthesis was investigated by reacting the two products to determine if conversion is possible. The phenol, methyl guaiacol, was not present in one set of reactions and was in excess in another. The reactions were followed by HPLC to determine the relative concentrations and rates of formation. It was found that an equilibrium exists between the two products and the phenol.

Soil Particle Size Analysis using the Dry Sieve Method. *Rosalie M. Ferri (Yakima Valley Community College, Yakima Washington 98902). Dr. Steve Reidel (Pacific Northwest national laboratory, Richland, Washington 99355).*
At the Hanford Site, one of the major problem is the storage of nuclear waste. How the waste is stored can have a significant impact on the environment. The radioactive waste stored at the site must not be allowed to reach the outside environment. Careful consideration is given to not only what type of containers to store the waste in, but also where to store the waste. In selecting a location for waste storage an important factor that is looked at is if the containers the waste is stored will leak and what will happen to the material that does leak out. A particle size analysis is done to determine the hydrological properties of the soil. In other words, how fast and at what volume will fluid materials seep through the soil? If ground water is flowing through the soil at a rapid pace, a small amount of waste leakage could be diluted so as that it does not cause an environmental problem. If on the other hand the waste is seeping through at a faster pace and of volume quantity that cannot be diluted, it will remain highly toxic and pose a hazard to the environment. The process of dry sieving the soil through a series of different size sieves will tell us the hydrologic properties of the soil at different depths. Calculating the percentage of gravel vs. sand vs. silt in the soil will enable us to do a computer model of a projected site and predict the hydrologic performance.

Evaluation of Chemical Transport in Soil Using Multimedia Environmental Fate Modeling. *Kirsten Enoch (San Francisco State University, San Francisco, CA 94132) Deborah Bennett and Thomas McKone (Lawrence Berkeley National Laboratory, Berkeley, CA 94720)*
Multimedia environmental models are used to understand the fate and transport of chemicals in multiple environmental media such as air, water, vegetation, soil, and sediment. Understanding the behavior of chemicals in the environment allows for the assessment of possible adverse effects on human and ecological health. Some multimedia fate models use the fugacity concept to describe the behavior of chemicals in environmental media. Multimedia models, such as CalTOX, are available for public use in order that exposure rates can be determined for populations in all areas. As one of the updates, a new user-friendly interface will be added to CalTOX. Recent research has provided new equations for the behavior of chemicals in soil and for chemical, landscape, and exposure factor data that will be added to CalTOX. These changes are assessed using four case studies: benzene, methyl tertiary butyl ether (MTBE), 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD), and benzo(a)pyrene. The CalTOX model produced similar data when compared to the collected data. Bioturbation was found to be an important factor in the new soil algorithms.

Grassland Water District Real-Time Water Quality Management and Panoche Drainage District Algal-Bacterial Selenium Removal System. *Adele Gelvin (Northeastern Junior College, Sterling, Colorado 80751). Nigel Quinn (Lawrence Berkeley National Laboratory, Berkeley, California 94720).*
Water quality is a common environmental concern that scientists are working to improve. Two current projects being conducted in the San Joaquin Valley of California are the Grassland Water District Real-Time Water Quality Management project and the Panoche Drainage District Algal-Bacterial Selenium Removal System project. The Grassland Water District project focuses on the concentration of salinity in the 90,000-acre wetland area and the amount that is released to the San Joaquin River in the spring. The high salinity is a problem for farmers in the early spring irrigation because the salinity interferes with water uptake by the plant which causes poor germination and growth, resulting in poor production. Panoche Drainage District Algal-Bacterial Selenium Removal System utilizes algae and bacteria to reduce nitrate and selenate found in tile drainage water. The project incorporates two pilot systems to determine the most effective and cost efficient system in which a larger plant can be built. The nitrate is a problem because it influences unwanted algae growth in the canals. The selenate poses a threat to waterfowl and their offspring by acting as a teratagen. My role was to

create a web page explaining the importance, location, and nature of each project. I also created a newsletter for the Panoche Drainage District.

Electrokinetics in the Bioremediation of Soil Contaminated with Nitroaromatics. *Stacy A. Green (The Ohio State University, Columbus, Ohio, 43210) John Kerr (Lawrence Berkeley National Laboratory, Berkeley, California, 94720).*
Through years of use as pesticides, in industry, and in the manufacture of munitions, nitroaromatics have contaminated the world's soil and groundwater. Recognized as priority pollutants, these compounds are known carcinogens and cause damage to the blood and to other internal organs. In the natural environment, small amounts of these substances can be broken down naturally into harmless, inorganic compounds and minerals. If the nitroaromatics are not fully degraded, however, they are converted into even more dangerous intermediates. When found in large concentrations, this is most often the case. Bioremediation is the most effective means of cleaning up nitroaromatics. Because the process uses microorganisms and is carried out on site, it is more efficient and costs less than the alternative dig-and-incinerate method. Electrokinetics enhances bioremediation by using electricity to deliver nutrients, water, and heat to the microorganisms. The application of electrokinetics is shown to have increased the rate of bacterial growth. When the microbial community grows, the rate of remediation is increased. Currently, only two countries worldwide, the United States and Germany, have assessed their levels of nitroaromatic contamination. Estimates indicate, however, that the levels of contamination elsewhere are high, making remediation of nitroaromatics an important global issue.

Polynuclear Aromatic Hydrocarbons in situ bioremediation treatability test; focus on contaminant disappearance by HPLC analysis. *Jessica Montañez[1], Loyda Méndez[1], Sadhana Chauhan[2], Terry C. Hazen[2]. [1]University of Puerto Rico Mayagüez Campus, Mayagüez Puerto Rico, [2]Ernest Orlando Lawrence Berkeley National Laboratory.*
Polynuclear Aromatic Hydrocarbons (PAHs) including Benzo(a)pyrene (BaP) are hydrocarbons containing two or more fused benzene rings. They are mostly found in the emissions from burned plant and petroleum products. One of the sites contaminated with PAHs is the United States Navy Base, Site 25 Parcel 182 at Alameda, CA. Biosparging, a bioremediation technique, is being considered for use at this site. This approach will allow the injection of air, methane, phosphorus and nitrogen to stimulate the indigenous microorganisms in the soil to increase their densities and degrade the PAHs. To establish that BaP in the soil at this site can be degraded by this technique, a treatability study is being done. Soil with no known pollution history was spiked with 10 ppm of BaP. These BaP and soil mixtures were amended with 10% methane (CH_4), 1% nitrous oxide (N_2O) and 1% triethyl phosphate (TEP). The total amount of CO_2 and CH_4 produced as a degradation product was quantified by gas chromatography (GC). Soil samples were extracted with acetone by vortex and sonication techniques. BaP recovery was quantified by High Performance Liquid Chromatography (HPLC). Vortexing was shown to be the best extraction method; however, the percent of extraction was low due to high BaP absorption to the soil. BaP concentrations decreased in every sample that contained CH_4, except for those amended with N_2O + CH_4 + TEP because it had a leakage. Unamended and CH_4 samples showed increases in biomass and microbial diversity in contrast with the amended samples, which showed low microbial density.

MTBE Remediation Via Co-Metabolic Degradation. *NICOLE PORTLEY (Boston College, Chestnut Hill, MA 02467) WILLIAM STRINGFELLOW (Lawrence Berkeley National Laboratory, Berkeley 94610)*
Methyl *tert*-butyl ether (MTBE), an oxygenate and gasoline additive, is a prevalent water pollutant in California. The first objective in this project was to learn basic microbiology techniques. These techniques were then applied to test the hypothesis that strains of bacteria may be able to degrade MTBE co-metabolically while receiving primary nutrition from another gasoline component. Bacteria strains were isolated and cultured from a field sample where MTBE degradation was quantifiably taking place. These bacteria were streaked upon a single-source media with *iso*-pentane, hexane, or octane as a carbon source. Thus, the bacteria were separated by their ability to live on certain hydrocarbons. Several cultures were tested via gas chromatography for MTBE degradation. Evidence shows that *iso*-pentane sustained bacteria are the best MTBE degraders.

Energy Efficient Fixtures for Real World Applications. *Laura Schloss (Gonzaga University, Spokane, WA 99258) Michael Siminovitch and Jeffrey Mitchell (Lawrence Berkeley National Laboratory, Berkeley, CA 94720).*
Improving energy efficient light fixtures is the primary goal of the Energy Efficient Lighting Laboratory. Various photometric techniques are implemented as a crucial element for the designing of energy efficient lighting technology. Currently, instruments such as a Gonio-Photometer and an Integrating Sphere are used for testing fixtures and bare lamps. A Downlight Integrating Chamber was built at minimal cost and will ultimately be capable of testing downlight fixtures for a greater variety of applications than current methods being used. Fixture controls are another important element of saving energy. A modified occupancy sensor was installed on the lighting system of a beverage machine which dims the machine's lights when no one is around. This Energy Smart technology saves energy without compromising the marketing technique of beverage machine companies. Using the energy efficient technology described herein will benefit the E.P.A. regulatory system, improve production for lighting manufacturers, improve marketing for beverage machine companies, and save millions of dollars in energy consumption.

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Clean Fractionation-A More Efficient Approach to Wood Pulping. *MATT BOOTH (Bismarck State College, Bismarck, ND 58501) JOE BOZELL (National Renewable Energy Laboratory, Golden, CO 80401)*
Wood pulping is an important process in industry because it produces cellulose, which is used to almost make everything from paper to plastics. However, while most of the current methods of wood pulping produce cellulose, they also lose the other chemicals in the wood. Clean fractionation is a new method of wood pulping that not only produces but also separates the lignin and the hemicellulose from the cellulose. This reaction is carried out inside a reactor, which is essentially a big stainless steel cylinder with heaters. Also, the clean fractionation method was developed at the DOE's National Renewable Energy Laboratory, and currently is a co-venture between the DOE and two companies. One company is Eastman Chemical, and it is a major cellulose consumer. The other company can't be named at this time, but it is a major cellulose producer. At this phase in the project, the major cellulose producer is looking to build a clean fractionation reactor of their own, but before they do they need a large quantity of pulped wood chips to study. So, over the summer, several runs were performed using the reactor at NREL, and the resulting wood chips were sent to the company to be tested. Next, those wood chips will be analyzed, and those results will be sent back to NREL.

Clean Fractionation-A More Efficient Approach to Wood Pulping. *NICOLE PASCHIS (Front Range Community College, Boulder, CO 80301) JOE BOZELL (National Renewable Energy Laboratory, Golden, CO 80401)*
The need for alternative sources for products is high. The National

Renewable Energy Laboratory in Golden, Colorado has dedicated its research to finding these sources. One such method has been carried out by using a renewable feedstock, wood, to research different ways to utilize the energy found within the layers of wood. To get these products which are in high demand, research has found that cellulose polymers are a source for products such as cellophane, drapery, latex paints, and tool handles. The Clean Fractionation process was developed to explore ways to obtain the purest and highest yield of cellulose. This process involves using solvents to obtain the three components of wood: lignin, hemicellulose, and cellulose, the latter being the main product of interest. A machine used, which is called a reactor, was designed to carry out this process. The reactor is made of a stainless steel tube, which contains wood chips and is used to heat and transport a solvent, which dissolves lignin and hemicellulose into an organic black liquor. This black liquor is then divided into its components by means of separation and distillation in a rotovaporator. The solvent used is made of methyl isobutyl ketone (MIBK), ethanol, water, and sulfuric acid. MIBK is the primary lignin dissolver, and exists as 16% of the solvent. Ethanol, comprises 33.8% of the solution, and is added to make the water and MIBK a single-phase solution. Water, as 49.9% of the solution, is added to dissolve the hemicellulose, or the sugars. And lastly, the sulfuric acid acts as the catalyst of the solvent. After the solvent is pumped through the reactor, the liquid product, the black liquor, containing the lignin and hemicellulose, and the solid product composed of primarily cellulose, result as the products of the reaction. This process promises an efficient way to extract cellulose.

Lung Cancer Assessment for Diesel Exhaust. *WENDY KIRCHOFF (University of Washington) Charlette Geffen (Strategic Planning, Pacific Northwest National Laboratory, Richland, WA 99352)*
Diesel exhaust is a complex mixture comprised of inorganic and organic compounds, some of which are known carcinogens and others probable carcinogens. Understanding the effects of these compounds on humans is important for associating lung cancer with diesel exhaust. The evidence of health effects from both diesel exhaust and the particulate matter associated with diesel exhaust are derived from extensive studies of animals, *ex vivo* and *in vitro* studies, and observations of various kinds of mutagenic studies. Research provides evidence of lung cancer in association with diesel exhaust, but both are subject to considerable uncertainty. Cellular studies present potential biomarkers of exposure to diesel exhaust that may play an important role in human lung cancer. Filling in the gap between exposure at the cellular level and the whole-body level are necessary in completing our understanding of diesel exhaust exposure and lung cancer.

Detection of Groundwater Contaminants by Propagation of Seismic Waves. *SHRAVANTHI REDDY and Dr. Ernest Majer (Mentor) Earth Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA)*
Propagation of seismic waves was used for the detection of contaminants known as DNAPL's, specifically PCE, a cleaning solvent that is now contaminating ground aquifers. Velocity analysis of the waves proved to be a useful technique for determining the presence of the contaminant in water-saturated sand and clay, in a tank sized model of a ground aquifer. Velocities of the waves decreased by as much as 5% in the presence of PCE. Amplitudes of the waves were also effected, experiencing significant attenuation in the presence of the contaminant. These techniques for detection of contaminants may be useful for more efficient remediation of groundwater aquifers.

MATERIALS SCIENCE

Redox of Simulated Nuclear Waste Glass Forming Melts. *Sara Vick (University of New Mexico, Albuquerque, New Mexico 87131) S.K. Sundaram (Pacific Northwest National Laboratory, Richland, Washington 99355).*
Glasses are found in the majority of reduction-oxidation (redox) items that are used everyday; from automobiles to planes, skyscrapers to apartment complexes. Because of the stability of most glasses, they are even being used to store hazardous waste materials. Many elements have different oxidation states and can be found in multiple states in the glasses. Redox of glasses has significant effect on processing of waste glass melts in melters as well as the properties of the waste forms. Nuclear waste glasses generally have complex chemistry (including several redox ions) and form corrosive melts. The basic objective is study the redox of the glasses containing Fe and Ni, using square wave voltammetry. We chose a basic simulated frit glass used for vitrification. The frit composition used was 57.90% SiO_2, 17.70%Na_2O, 14.70%B_2O_3, 5.70% Li_2O, 2.00% MgO, 1.00% TiO_2, 0.50% ZrO_2, and 0.50% La_2O_3. The batch glasses were synthesized and then dopants of Fe_2O_3, NiO, and a combination of Fe_2O_3-NiO were added in 1-wt % amounts. The glass was then melted at 1150° C and held for 24 hours. It was then poured to the top of a medium sized Pt/Rh crucible and placed in a furnace at 1150° C. The glass powder was allowed to melt for five minutes before the testing apparatus was placed in the melt. The testing apparatus was composed of a Pt/Rh working electrode, Pt/Rh counter electrode, and a Zr/Al reference electrode. The counter electrode is placed in the melt until it is touching the bottom of the crucible creating a closed circuit. Both the reference electrode and the working electrode are located half way down the counter electrode. The test showed that melt resistivity was high which indicates the amount of conductivity in the melt. Sample melt volume and area of the working electrode were high. Adjusting the crucible size and sizing other electrodes will improve the measurements. Future work includes testing on the NiO glass and the Fe_2O_3-NiO glass to see the interaction between the Fe and the Ni and synthesis of 2 wt %, 3 wt %, and 5-wt % Fe_2O_3 doped glasses to further study the effect of Fe concentration.

Aqueous-Based Latex Systems for Producing Durable Waste Forms-Initial Characterization. *Troy Terry (Montana State University, Bozeman, MT 59715) R. Russell, H.D. Smith, L. Liang, G.L. Smith (Pacific Northwest National Laboratory, Richland, WA 99352)*
The overall objective of this project is to identify and successfully demonstrate a water-based polyceram system suitable for producing an environmentally stable waste form highly loaded with salt wastes. The backbone for this idea is the development of aqueous based sol-gel technology. Most interest in sol-gel synthesis of ceramics in recent years has concentrated on the hydrolysis of metal alkoxides in organic media, but the alternative sol-gel process in aqueous media may offer acceptable results without the need for hazardous precursors or waste products. To accomplish this, water micelle (like an emulsion) systems will be substituted for the organic based systems already identified. Preliminary tests show that emulsions such as Styrene/Butadiene and Acrylic latex are good candidates for the aqueous media. Both of these materials when mixed with a percentage of natural latex have been shown to effectively immobilize salt wastes with loadings over 10 wt%. The low cost, availability, and ease of preparation (low temperature of cure) of these products makes them strong contenders as a waste form. Techniques for improving both chemical and physical properties, such as adding cross-linking agents and fine-tuning the curing process, are currently in development at Pacific Northwest National Laboratories along with collaboration with staff from the University of Arizona.

Thermal and Mechanical Damage Characterization of Advanced Ceramic Materials. *JEREMY JONELIS (University of Illinois, Urbana, Illinois 61801). BALAKRISHNAN G. NAIR (Argonne National Laboratory, Argonne, Illinois 60439)*
Thermal and mechanical damage characterization of a variety of material systems, including refractories, thermal barrier coatings, and nano materials, were studied. The insulating refractory material in steelmaking furnaces is subjected to corrosion/erosion by slag attack. These refractories were evaluated under a variety of conditions to determine optimal compositions and conditions for refractory usage. Thermal barrier coatings (TBCs) allow conventional superalloys in engines and turbines to be used at higher temperatures. However, stresses induced from exposure to high temperature cause nucleation and propagation of microcracks in the ceramic, reducing the life of the material. Work centered on measuring hardness and elastic modulus of TBCs to monitor microcracking as a function of exposure time. Nanophase alumina powders with high surface area have the potential to be used in catalytic applications and as reinforcements in composites. Commercial nanophase alumina powders consist of a metastable ?-phase. Current work concentrated on (1) studying the phase stability of alumina powder, and (2) identifying optimal heat-treatment parameters for the formation of a stable nanophase ?-alumina powder.

Study of Grain Boundaries in YBCO Superconducting Films. *RYAN MUNDEN (Stetson University, DeLand, FL 32720) PETER BERGHUIS (Materials Science Division, Argonne National Laboratory, Argonne, IL*

60439)
Current interest in high temperature superconductors (HTS) has warranted much research into their properties. Many difficulties exist in applying these ceramic-like superconductors in technological and scientific uses. Many manufacturing techniques attempt to eliminate these difficulties, especially those that limit the critical current density, Jc, of the superconductors. Great efforts are made to assure that the grains of the superconductor are all aligned, providing a high Jc. One of the greatest difficulties is the presence of grain boundaries, regions where the grains of the superconductor suddenly shift orientation by several degrees. These grain boundaries introduce little understood effects into the behavior of the bulk superconductor. By evaluating thin films of $YBa_2Cu_3O_7$ (YBCO) with a grain boundary of well defined misorientation angle it is hoped that a better understanding of their effects can be determined. Low angle grain boundaries can increase Jc through improved flux pinning. High angle grain boundaries can greatly degrade Jc by causing high current dissipation due to increased flux flow. Through current-voltage measurements over a broad spectra of magnetic field and temperature conditions, the effects of a low angle grain boundary in an YBCO film are examined.

Methods for studying the interactions between proteins and mineral substrates. *LINDSEY VANSCHOIACK (Rose-Hulman Institute of Technology) Allison A. Campbell, Ph.D. (Battelle Pacific Northwest National Laboratory, Richland, Washington 99355)*
The importance of protein and mineral interactions in subsequent mineral growth; the change that adsorbed proteins cause in the mineral's natural properties are currently of interest in many fields of study. This paper deals with the effect of bovine serum albumin (BSA) adsorption on hydroxyapetite's (HAP) natural growth rate. The effect that adsorbing Protein G (Pro G) on calcium oxalate (CaOx) has on that mineral's mobility in several concentrations of sodium chloride (NaCl) solution was also examined. The methods used to quantify this data include: UV-Visible spectroscopy, particle characterization instrumentation capable of measuring zeta-potential, and constant composition kinetics (CC) titration. The protein was adsorbed by the two minerals for one hour and the resultant growth rate and charge data was compared to the data from the minerals in the absence of protein. The background electrolyte was varied through three ionic strengths with various results. The resultant data supported previous work already obtained in several areas and posed several new and interesting results that will be the subject of future research.

Development of Shearography Technology for Nondestructive Characterization of Materials. *LEONARDO MELO (Richard Daley Community College, Chicago, Illinois, 60652). William Ellingson (Argonne National Laboratory, Argonne, Illinois).*
Shearography is a method of nondestructive testing that measures surface strains on the materials tested through the analysis of the speckle pattern. In shearography, a laser beam is used to illuminate the sample being tested and CCD camera captures that image. Before the image is captured by the camera, a shearing device, in my case a Wollaston prism, is set up in front of the camera, which produces a pair of sheared images that are captured by the camera, hence the name shearography. The shearography lab has not yet been completely set up because of unexpected problems faced along the way. Adjustments have been made so that those problems can be fixed and the setting up of the lab can continue. Results proving that the current set up does work, have been gathered. There are problems related to using the current set up which prove that this set up needs to be improved or changed for performing the shearography lab.

Molecular Magnets: Synthesis and Characterization. *JANA LECHER (Hanover College, Hanover, IN 47243) DR. JAMIE L. MANSON (Argonne National Laboratory, Argonne, IL 60439).*
Magnetic materials are an essential part of modern life and are important to the advancement of certain scientific fields. An attempt is underway in materials science to synthesize magnetic materials either partially or completely out of organic molecules. Such materials have several distinct properties to offer over traditional magnets. The syntheses of several such materials of formulas $[M^{+2}(HCO_2)_2L]$ [M = Mn, Fe, Co, Ni, Cu, Zn; L = pyrazine, pyrimidine] and $[M^{+2}(HCO_2)_2L][M$ = Mn, Cu; *L* = substituted pyrazines and pyridines] were attempted using wet chemistry techniques. For certain reactions the order of addition of reactants was varied while other reactions were carried out in different solvents to better understand the nature of the reactions taking place. The materials were characterized using infrared spectroscopy (IR), X-ray diffraction, and DC magnetization. According to preliminary analysis of IR data for the $[M^{+2}(HCO_2)_2L]$ series, compounds containing all three components when L = pyrazine include M = Co, Ni, Cu, Zn. When L = pyrimidine, successful syntheses appear to have been achieved for M = Co, Ni, Cu. For the $[M^{+2}(HCO_2)_2L]$ series where *M* = Mn, all three reactants are present in only three of sixteen attempted syntheses, and for the same series where *M* = Cu, data has been recently acquired but its analysis is not yet complete. Some X-ray diffraction and DC magnetization data has also been recently received but its analysis is not yet complete. The final week of this study will be devoted to interpretation of available data.

The Mechanics of Fluids and Heat Transfer. *Libny D. Pineda (South Texas Community College, McAllen, TX 78502) Jeff Collins (Argonne National Laboratory, Argonne 60439).*
The Advanced Photon Source (APS) is one of the newer buildings found at Argonne National Laboratory where a beam line is the main resource used. The beam is a collection of electrons shot by an electron gun at nearly the speed of light. This beam is ten times hotter than the surface of the sun yet is only about one mm in diameter. The idea is to cool down the beam when it strikes a surface. There are blocks of massive Tungsten metal placed in the path of the beams that are tangent to the main beam. These tangential beams overheat tremendously when they hit or strike these surfaces. The Tungsten metal which is being used, is a very massive metal with high heat capacity. Each Tungsten block has a hole all the way through to allow hoses to run through it. These tube/hoses run water through them with porous media inside, transferring nearly all of the heat away from the Tungsten. The porous media is placed in a tube and water is pumped through at 100 psi. The Advanced Photon Source users plan to turn the power up on the beam from 200 mA to 300 mA. This however, tends to causes even more heat to build up so that some of the heat is non-transferable. The tungsten block has a problem of losing mass exponentially on a day-to-to day basis. Utilizing an $80,000 infrared camera to simulate and to study the strike surface of the beam, resulted in new discoveries being determined of the structural integrity of Tungsten.

Electrophoretic Deposition of Functionally Graded Materials. *JERAMY ZIMMERMAN (Colorado School of Mines) Will Windes (Idaho National Engineering and Environmental Laboratory, Idaho Falls, Idaho 83415*
This summer I have been working on creating a system and determining the parameters to deposit a functionally graded material that changes from 100% Ni at one surface to 100% alumina on the other surface in one continuous gradient. This deposition has been carried out in an

ethanol suspension with $MgCl_2$ and water additions to increase deposition rate and adherence. Deposits have been deposited in thickness exceeding 1 mm in thickness and have been made in a variety of increment compositions including up to 5 layer deposits. The project is currently at the stage that a device is being made to create the continuous gradient.

Testing of stainless steel 304L/SA210 tubing under thermal and stress variations. *SAMUEL PEPI (University of Texas at Brownsville, Brownsville, TX 78521) Christopher Stevens (Oak Ridge, TN 37831).* Cracking of stainless steel 304L/SA210 carbon steel tubing, which is used in Black Liquor Recovery Boilers, has become a concern in paper mills both in the United States and abroad. The majority of the incidents have involved cracking in the outer 304L stainless steel layer. Although evidence of pitting in the SA210 carbon steel has also been observed, the cracking has not continued into the SA210 carbon steel. However, the propensity for cracking to penetrate the SA210 carbon steel is a cause for concern. As part of this study, the pipes will be tested in an environment that resembles the conditions that exist in the paper mills as closely as possible. The tubes will undergo thermal fluctuations and stresses in order to pinpoint the material's specific deficiency. This will be achieved by placing tubes of 304L/SA210 in a Teflon sleeve containing Na S (sodium sulfide), a corrodent, and then doing load testing. Heating tape is placed along the inner portion of the tube that is exposed to the corroding agent, and the tube is heated to 200°C. This procedure closely replicates the environment in the paper mills and, provides a way to closely monitor the reaction of the tubes.

Hydroxyapatite Nucleation on Various Substrates Using the Biomimetic Process *DANIEL SHINOBU STEVENS (University of Washington) Dr. Allison A. Campbell (Environmental and Health Sciences Division of Battelle Pacific Northwest National Laboratory, Richland, Washington 99352)*
The biomimetic process is currently used to coat bone implants with hydroxyapatite (HAP). HAP is the phase of calcium phosphate which is predominately found in human bones and teeth. Furthermore, it also constitutes the majority of inorganic compounds in both of these structures. This fact has prompted further research into maximizing the efficiency of this process. HAP coatings were grown on silicon wafers, titanium wafers, and various ion-exchange resins using the biomimetic process. This technique modifies the surface of the substrate and allows the surface functionality to be chosen. Next, the samples were placed in supersaturated calcium phosphate (CaP) solutions to promote HAP surface nucleation and growth. X-ray diffraction spectroscopy (XRD), Fourier transform infrared spectroscopy (FTIR), contact angle measurements, and scanning electron microscopy (SEM) were used to characterize the coatings. Inductively coupled ion plasma spectroscopy (ICP) was used to determine calcium and phosphate ion concentrations in the solutions, and ultimately the rate of CaP adsorption. By comparing the rates of CaP adsorption for surfaces with different functionalities, the functionality that promotes the fastest rate of CaP adsorption can be determined.

Carbon Fiber Composite Fabrication and Enhanced Fiber Interfaces. *Brian True (Washington State University, Richland, Washington, 99352) K.L. Simmons (Pacific Northwest National Laboratory, Richland, Washington, 99355)*
The U.S. Army Armament Research Development & Engineering Center (ARDEC) sponsored this research project to support the development of new self-assembled monolayer fiber coatings. These coatings can greatly increase the bond strength between the fiber and the resin matrix of a composite material. Composite munitions components molded from such materials will exhibit higher strength than current materials, and will provide a major improvement in the performance of composites in military applications. Use of composite materials in military applications is desirable because of the lighter weight of the materials and their high strength. The objective for the proposed project Carbon Fiber Composite Fabrication and Enhanced Fiber Interfaces is to chemically modify the surface of carbon fiber with Self-Assembled-Monolayers (SAMs) for enhancing the strength at the interface to polyetherimide thermoplastic matrix resin. The project will demonstrate how to develop commercially viable surface chemistry methods (most notably SAMs) and how those modifications can improve the adhesion between the polymer phase and the fiber. The project will also demonstrate at what rate SAMs can be applied using a commercial system. The mechanical properties testing, e.g. flexural, short-beam shear, tensile and compressive strengths, will be used to determine how well the SAMs enhance mechanical properties through the surface modifications at more desirable rates for commercialization. An industrial partner will be brought into the program to help improve production speeds of the SAM processing. The deliverable will be results of the research and testing in a PNNL published report and journal article(s).

The Effect of Gadolinium on Hafnium Solubility in Peraluminous and Subaluminous Glasses. *Leslie Dalbey (University of Montana, Missoula, MT 59812) L. Davis, J. Darab, D. Strachan (Pacific Northwest National Laboratory, Richland, WA 99352).*
The effect of gadolinia (Gd_2O_3) on the solubility of hafnia (HfO_2) was determined for peraluminous and subaluminous glasses ($Al_2O_3 \geq Na_2O$) in a borosilicate system. Gadolinia and HfO_2 are being considered as surrogates for Pu(III) and Pu(IV) respectively in waste glass. In the U.S., some Pu may be incorporated into glass. Preliminary studies conducted with Gd_2O_3 and HfO_2 allow predictions regarding the behavior of Pu(III) and Pu(IV) in glasses and the behavior of neutron absorbers (e.g., Hf and Gd) with Pu. Hafnia solubility was determined for base glasses containing the following: ~60 mole % SiO_2; ~15 mole % B_2O_3; a peralkalinity ratio (PL), $Na_2O/(Na_2O+Al_2O_3)$, from 0.0 to 0.5; and 0, 2, 4, 10, 11.5, or 34 mole % Gd_2O_3. The HfO_2 solubility limit was defined as the composition at which Hf-bearing crystals are detected by use of a high-powered optical microscope. For all glasses except that with PL equal to 0.45 and containing 2 mol% Gd_2O_3 (i.e., PL0.45Gd2), the only Hf-bearing phase to crystallize was HfO_2; whereas, in PL0.45Gd2, (Hf,Gd)O2 crystallized in addition to HfO_2. Hafnia solubility increased with increasing Gd_2O_3 content in the base glass. For example, for PL0.50 with 0, 2, and 4 mol% Gd_2O_3, the solubility limit of HfO_2 was 1.99, 2.92, and 3.71 mole %, respectively. In conclusion, increasing the Gd_2O_3 content in the base glass increased the HfO_2 solubility. Therefore, Gd_2O_3 may be used as a neutron absorber and as a means of increasing the solubility of PuO_2.

Lanthanide and Actinide Extraction Using Cyanex 272. *Christopher Linrud (Oregon State University, Corvallis, Oregon, 97331) Mark Jensen (Argonne National Laboratory, Argonne, Illinois, 60439).*
Nuclear waste is a growing problem in society today. If nuclear power is to be used in the future, a way must be found to reduce the amount of radioactive waste. The extraction of the lanthanide and actinide elements from nuclear waste may be part of the solution. Cyanex 272 was studied to determine the distribution ratios for the lanthanide series, excluding Pm, along with Am, Cm, and Cf. The distribution ratios were found by Arsenazo III spectrophotometery for the lanthanide elements

and by activity for the three actinides. The lanthanide series provided an average discrimination in distribution ratios of around 1.6.

Correction of Oligonucleotides in a Complete Six-mer Library Arrayed on Polyacrylamide Gel Pads. *Tamara Nelson (Austin Community College, Austin, Texas, USA 78703) G. Yershov (Argonne National Laboratory, Argonne, Illinois 60439).*
Manufacturing of microchips was performed in order to test oligonucleotides arrayed on a Generic Chip. It was discovered that 9 of 4,064 oligonucleotides in a complete six-mer library did not give anticipated results upon hybridization with a sample sequence. One of the questioned oligonucleotides is compared to a newly synthesized oligonucleotide of the same sequence by means of hybridization. The immobilization procedure was also checked in order to verify proper immobilization of the oligonucleotides. It was discovered that the immobilization procedure was carried out correctly. As for the hybridization results, it was determined that the new oligonucleotide gave a higher signal, but the same experiment must be repeated because the signal is not intense.

MEDICAL & HEALTH SCIENCES

Information Management Approach to the Virtual Human. *JOY E. WRIGHT (Christian Brothers University) of Dr. Richard Ward and Kara Kruse (Computational Physics and Engineering Division at Oak Ridge National Laboratory Oak Ridge, Tennessee 37831-6064)*
The Virtual Human Project has the vision of structuring the complete human body with working organs and body functions to appear on computers to aid in medical diagnosis. Towards this goal, researchers at ORNL have developed a Java client/server architecture for linking physiological models written in various programming languages. This architecture takes advantage of Java Remote Method Invocation (RMI) to connect a Java client-user interface to servers where the physiological simulation codes reside. Forms for describing the models were created using XML (Extensible Markup Language) documents to describe the model variables, parameters and initial conditions for each model. A DTD (Data Type Definition) file was used to control the information being entered on the web-based forms that were created using Java applets. The information was retrieved and stored in a database using JDBC (Java Database Connectivity). The forms are needed to assist the users of the various models in entering the appropriate information to start the different simulations. They will also help keep control of administration's accessibility to change relevant data structure and default values to the models. The main purpose of using XML and DTD in creating forms is to provide a very flexible, modular, distributed environment where the model, model data, and user interface are separated. Such an environment allows the rapid modification of current models and integration of new models into the environment.

Daily Exposure to Ambient Particle Matter (PM-2.5) and Our Health. *AMY FELDMAN (Valdosta State University, Valdosta, Georgia 31602) MELISSA LUNDEN (Lawrence Berkeley National Laboratory, Berkeley, California 94720).*
Understanding the role that ambient particle matter has on our health is of significant importance. The population is exposed to these suspensions of solid or liquid particles known as aerosols on a daily basis. Epidemiological studies have found correlations between exposure to "inhalable particles" (particle matter less than 2.5 micrometers in diameter, PM-2.5) and increased mortality rates and other adverse health effects. Yet, not much is understood about why these inhalable particles are harmful to humans. We do not know whether the specific species present in particle matter or total particle mass is harmful. The amount of PM-2.5 to which people are exposed is also still unknown. This is because people spend, on average, 85-90% of their time indoors, while pollutant measurements are performed outdoors. The purpose of our four phase research project is to develop a semi-empirical mathematical formula to detect concentrations of PM-2.5 indoors based on outdoor measurements. This information is crucial to understanding the role that these "inhalable particles" play in affecting our health.

Preparation for X-Ray Crystallography of the AZU-1 Candidate Breast Tumor Suppressor Protein. *HELENA LEE (Harvard University, Cambridge, Massachusetts 02138) LI-WEI HUNG (Ernest Orlando National Laboratory, Berkeley, California 94720)*
Tumor suppressor proteins act as negative controls on the cell growth cycle, inhibiting the uncontrolled proliferation of cancer cells and activating cell death. AZU-1, which is a candidate for a breast tumor suppressor protein, is found in levels much lower in tumorigenic cells than in non-cancerous counterparts. Using x-ray crystallography techniques, the structure of the AZU-1 protein can be determined as a three-dimensional model. The folding structure and the spatial relationship of the protein domains can be compared to known protein structures, and the specific molecular function of AZU-1 is subsequently inferred. This inferred molecular function provides more information on the cellular role of AZU-1, which is essential knowledge in the design of drugs to promote protein performance. To prepare for x-ray crystallography, the AZU-1 protein gene was cloned into bacterial pET vector systems in four different constructs of varying sizes to optimize expression and solubility for eventual purification and crystallization. The over-expression of the full-length protein construct yielded high over-expression of only the vector tag, indicating incomplete digestion and transformation. The solubility of the protein expressed was increased through lowering induction temperatures and increasing times. Current work is being done on smaller construct sizes isolating separate AZU-1 domains in cloning and over-expression.

In Search of Beta Catenin: A Look at Protein Localization in Breast Cancer Cells. *Elizabeth Taglauer (Southwest Missouri State University, Springfield, MO 72673), Carolyn Larabell (Lawrence Berkeley National Laboratory, Berkeley California, 94720), Deborah Yager (Lawrence Berkeley National Laboratory, Berkeley California, 94720).*
The Biological Microscopy Lab of Carolyn Larabell is currently using a cellular approach to better understand the nature of breast cancer. One of the research projects focuses on the nuclear localization of the cellular protein b-catenin. b-catenin is involved in two main functions: cell-cell adhesion and signal transduction during embryogenesis. During the non-cancerous functioning of a breast cell, b-catenin levels in the cytoplasm are regulated. When a breast cell transforms from a cancerous to a non-cancerous state, b-catenin can accumulate in the cytoplasm and enter the nucleus to turn on certain genes. There are currently varying hypotheses about the cause of the cytoplasmic accumulation and nuclear localization of b-catenin. In the Larabell Lab, immunocytochemistry-labeling techniques are being combined with confocal and soft X-ray microscopy techniques to study the cytoplasmic accumulation and nuclear localization of b-catenin within cancerous and non-cancerous breast cells.

Lung Cancer Assessment for Diesel Exhaust. *WENDY KIRCHOFF (University of Washington) Charlette Geffen (Strategic Planning, Pacific Northwest National Laboratory, Richland, WA 99352)*
Diesel exhaust is a complex mixture comprised of inorganic and organic compounds, some of which are known carcinogens and others probable carcinogens. Understanding the effects of these compounds on humans is important for associating lung cancer with diesel exhaust. The evidence of health effects from both diesel exhaust and the particulate matter associated with diesel exhaust are derived from extensive studies of animals, *ex vivo* and *in vitro* studies, and observations of various kinds of mutagenic studies. Research provides evidence of lung cancer in association with diesel exhaust, but both are subject to considerable uncertainty. Cellular studies present potential biomarkers of exposure to diesel exhaust that may play an important role in human lung cancer. Filling in the gap between exposure at the cellular level and the whole-body level are necessary in completing our understanding of diesel exhaust exposure and lung cancer.

The Application of the List Mode Likelihood Reconstruction to Positron Emission Mammography. *Tahinde Frederick (Hamilton College) Dr. Ronald H. Huesman (Lawrence Berkeley National Laboratory, Berkeley, California, 94720) and Bryan W. Reutter (Lawrence Berkeley National Laboratory, Berkeley, California, 94720).*
At the Center for Functional Imaging, researchers are currently building the Positron Emission Mammography (PEM) Camera, an alternative to x-ray mammography. In the process of reconstructing images, they have employed the mathematical methods of maximum likelihood and an iterative technique known as the EM Algorithm. In conjunction with these methods, they have used existing mathematical equations for the Gaussian Prior in an attempt to produce smoother images. In my research, I will derive the mathematical equations for using the gamma prior instead.

Evaluation of Fracture Resistance and Toughness of the Bovine Dentin-Enamel Junction. *JAMES HO (University of Illinois – Urbana-Champaign, Urbana, IL, 61801) ANTONI TOMSIA, JAMES MCNANEY (Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, 94720)*

Teeth, as the main component of our masticatory apparatus, undergo great stress and wear throughout their lifetime. It is our objective to understand the role the dentin-enamel junction (DEJ) plays in resisting crack growth and subsequent failure of the tooth. To go about this, we quantified its fracture toughness by creating DEJ samples and fractured them via a four-point bending test. A crack was initiated in the sample by creating a triangular notch near the DEJ. We observed the growth of the crack through a light microscope in between loading cycles. As only one sample has been completely fracture-tested, the data is inconclusive. Our end goal is to assist bioengineers in modeling the DEJ by providing them needed experimental data on its fracture behavior.

NUCLEAR SCIENCE

Characterization of the Metallic Uranium Spent Nuclear Fuel Colloids. *ANGEL CHAN (Western Illinois University, Macomb, IL 61455) Carol Mertz (Argonne National Laboratory, Argonne, IL 60439)*

The U.S. Department of Energy has proposed Yucca Mountain, NV, as the only candidate site for permanent disposal of high-level radioactive waste. The general goals of nuclear waste disposal are immobilization and geological isolation. Radionuclides can exist as dissolved ionic species and colloids or adsorb to colloids in the groundwater. Radionuclides bound to colloids can be present in solution in concentrations that exceed their chemical solubility. Thus site characterization of the potential transport of radionuclides colloids in the groundwater is a potential interest. In this project, several clay mineral colloids (Na-montmorillonite, kaolinite, and brick clay) and an actinide surrogate (cerium phosphate, $CePO_2$) were characterized by dynamic light scattering to determine their morphology and size distribution. The clay colloids exist predominantly as flat discs whereas $CePO_2$ has spherical shape. The individual colloids have a hydrodynamic diameter of ~2-5 nm and their aggregates have dimensions of ~50-250 nm. The corrosion behavior of N-reactor unirradiated metallic uranium fuel in a groundwater simulant was also examined. The uranium oxide corrosion product exhibits trimodal size distribution (mean diameters of approximately 5 nm, 150 nm and 750 nm). The colloidal analyses were conducted by dynamic light scattering, transmission electron microscopy, and scanning electron microscopy.

Delivery of Cryogenically Frozen Pellets Through Curved Guide Tubes for the Fueling of Fusion Plasmas. *Adam Griffith (Rice University, Houston, TX 77005) S.K. Combs (Oak Ridge National Laboratory, Oak Ridge, TN 37830).*

The physics and technology behind magnetically confined fusion have been developed greatly over the last three decades. A stumbling block in that development has been the issue of maintaining a high core plasma density. Being able to efficiently refuel a plasma is essential for the development of sustainable, long-term fusion reactions. The most promising refueling method is that of pellet injection. H_2, D_2, T_2, and D-T pellets on the order of one to a few millimeters at about 10 K are injected at high speeds (100 to 4000 m/s) into plasmas that can be 200 million K or more. Originally, pellets have been injected directly into the outer rim of the doughnut-shaped plasma. Vertical and inner-rim or high-field side (HFS) launches have also been tested, with improved plasma penetration and fueling efficiency. However, HFS injection requires the use of curved guide tubes, which exert forces on the pellet that tend to erode and break the pellets, dramatically reducing the pellet's ability to deposit fuel into the core of the plasma. This study aims to expand the base of knowledge associated with pellet injection by studying the survivability of hydrogen, deuterium, and neon pellets of 2.7 mm diameter when injected into either a single- or multi-loop guide tube. The data from this experiment will be used to assist in the design of more reliable curved guide tube systems and develop computer models that that will direct future pellet injector system designs.

My Participation in the Design of the KamLAND Detector *BRIAN ROEDER (Michigan State University, East Lansing, Michigan, 48824) KEVIN LESKO (Lawrence Berkeley National Laboratory, Berkeley, California, 94720).*

KamLAND (Kamioka Liquid Scintillator Anti-Neutrino Detector) is currently under construction in Japan and scheduled to be operational in the spring of 2001. KamLAND will be used to study the anti-neutrinos emitted by nuclear power plants in Japan and later to study the neutrinos emitted from the sun. The importance of these experiments will be to determine if neutrino oscillations exists and ultimately if neutrinos have mass. These results will have important consequences for the Standard Model for describing and identifying elementary particles. An important part of the US collaboration in the design and building of this detector is designing the Calibration System. In order to understand how the detector responds to different data events, these events will need to be simulated within the detector periodically. A computer controlled motion control system needs to be designed, programmed, and tested in order to lower various event-causing sources into the detector sphere, (radioactive sources, light sources, etc.). This motion control system has been designed and has been purchased, and is currently being tested. When the motion control system is finished, the mechanical part of the Z-Axis Calibration System can then be designed. It is also important to determine what materials are compatible with pseudocumene, part of the liquid scintillator mixture that is corrosive, so that materials eroded by pseudocumene are not used in the construction of detector components.

PHYSICS

The Mechanics of Fluids and Heat Transfer. *Libny D. Pineda (South Texas Community College, McAllen, TX 78502) Jeff Collins (Argonne National Laboratory, Argonne 60439).*

The Advanced Photon Source (APS) is one of the newer buildings found at Argonne National Laboratory where a beam line is the main resource used. The beam is a collection of electrons shot by an electron gun at nearly the speed of light. This beam is ten times hotter than the surface of the sun yet is only about one mm in diameter. The idea is to cool down the beam when it strikes a surface. There are blocks of massive Tungsten metal placed in the path of the beams that are tangent to the main beam. These tangential beams overheat tremendously when they hit or strike these surfaces. The Tungsten metal which is being used, is a very massive metal with high heat capacity. Each Tungsten block has a hole all the way through to allow hoses to run through it. These tube/hoses run water through them with porous media inside, transferring nearly all of the heat away from the Tungsten. The porous media is placed in a tube and water is pumped through at 100 psi. The Advanced Photon Source users plan to turn the power up on the beam from 200 mA to 300 mA. This however, tends to causes even more heat to build up so that some of the heat is non-transferable. The tungsten block has a problem of losing mass exponentially on a day-to-to day basis. Utilizing an $80,000 infrared camera to simulate and to study the strike surface of the beam, resulted in new discoveries being determined of the structural integrity of Tungsten.

Design and Characterization of an Effusive Flow Measurement Apparatus. *WHITNEY KATE ORTMAN (Juniata College, Huntingdon, PA 16652) R.F. Welton and M.A. Janney (Oak Ridge National Laboratory, Oak Ridge, TN 37831)*

Accelerated radioactive ion beams (RIBs) are becoming a vital tool in the study of the structure of the nucleus, astrophysical phenomena and material science. Several large scale facilities devoted to the production and utilization of these beams are operational worldwide while higher intensity RIB facilities are being planned for the near future in the United States and Europe. The Holifield Radioactive Ion Beam Facility (HRIBF) at ORNL is currently the principle RIB facility in North America. In the RIB production process, one the principle limitations of the intensity of RIBs is the physical and chemical interactions which occur between the radioactive atom and surfaces of the production device. If these delay times are longer with repect to the half-life, serious losses will occur. A new technique is being developed whereby these interactions can be characterized using stable analogues of the radioactive atom in an off-line, stand alone, thermal chromatographic apparatus. The time profile of the permeation of a gas or vapor passing through a high temperature ($1000°C < T < 2000°C$) column constructed from the material under investigation is measured. Kinetics of the atom-surface interactions are deduced from these data. This report details the design of various components of the test stand and describes initial flow measurements made using a wide mass range of noble gases through the column.

Vacuum Assisted Photoionization and the Advanced Light Source. *HANNAH S. ABEND (Queens College, Flushing, NY, 113670) DR. ALI BELKACEM (Atomic Physics Group, Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720).*

Vacuum assisted photoionization removes an inner shell electron through the creation of an electron-positron pair. Pair creation occurs when an incident high energy photon, at least twice the rest mass of an electron, approximately 1 MeV, interacts with the strong electric field surrounding the atomic nucleus and ceases to exist, creating in the process an electron-positron pair. Once a pair is created it will interact with an inner shell electron in its surroundings and expel it, causing the atom to ionize This process, known as vacuum assisted photoionization, has only recently been predicted and theorized about and no experiments have yet tested it. My mentor and his collaborators anticipate that the cross section of vacuum assisted photoionization increases at high energies, when the energy of the incident photon reaches at least twice the rest mass of an electron. We have constructed a beamline at the Advanced Light Source of the Lawrence Berkeley National Laboratory to test this theory. The primary motivations for the research are to better understand the dynamics and relationships between bound electrons and electrons from the QED vacuum.

Delivery of Cryogenically Frozen Pellets Through Curved Guide Tubes for the Fueling of Fusion Plasmas. *Adam Griffith (Rice University, Houston, TX 77005) S.K. Combs (Oak Ridge National Laboratory, Oak Ridge, TN 37830).*
The physics and technology behind magnetically confined fusion have been developed greatly over the last three decades. A stumbling block in that development has been the issue of maintaining a high core plasma density. Being able to efficiently refuel a plasma is essential for the development of sustainable, long-term fusion reactions. The most promising refueling method is that of pellet injection. H_2, D_2, T_2, and D-T pellets on the order of one to a few millimeters at about 10 K are injected at high speeds (100 to 4000 m/s) into plasmas that can be 200 million K or more. Originally, pellets have been injected directly into the outer rim of the doughnut-shaped plasma. Vertical and inner-rim or high-field side (HFS) launches have also been tested, with improved plasma penetration and fueling efficiency. However, HFS injection requires the use of curved guide tubes, which exert forces on the pellet that tend to erode and break the pellets, dramatically reducing the pellet's ability to deposit fuel into the core of the plasma. This study aims to expand the base of knowledge associated with pellet injection by studying the survivability of hydrogen, deuterium, and neon pellets of 2.7 mm diameter when injected into either a single- or multi-loop guide tube. The data from this experiment will be used to assist in the design of more reliable curved guide tube systems and develop computer models that that will direct future pellet injector system designs.

Investigation of the Parameters Affecting Current in the Electrospray Ionization Source. *HILARY A. SIDERS (Winthrop University, Rock Hill, South Carolina, 29732) DR. GARY J. VAN BERKEL (Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831)*
Electrospray ionization is a highly useful technique by which ions in solution can be transferred intact to the gas phase for mass spectral analysis. By its nature, the electrospray ion source acts as a controlled-current electrochemical cell, and thus can create ions from neutral electroactive molecules in solution. These ions may hinder or help the detection of the analyte ions, depending on the experiment and properties of the analyte and matrix solution. The electrochemical reactions that may form these "excess" ions depend in part upon the magnitude of the current across the gap between the emitter and the counter electrode. This means that a fundamental understanding of what parameters influence this current is necessary to fully understand and control these electrochemical reactions. This project was a systematic study of the three main parameters affecting the current: the flow rate, the magnitude of the electrical field imposed at the emitter tip and the conductivity of the solution itself. The data shows that the influence of each variable on the current is dependent upon the values of the other two experimental parameters. In addition, it was seen that the electrical field influenced the current magnitude more than the flow rate or the conductivity.

Advanced Light Source—An Advanced Form of Illumination: Photoionization of Acetylene. DIANA *BULL (Vassar College, Poughkeepsie, NY 12604) FRED SCHLACHTER (Lawrence Berkeley National Laboratory, Berkeley 94720)*
Fluctuations in the earth/atmospheric radiation balance are, in part, controlled by the interaction of molecules with each other and with radiation from the sun. In order to understand the outcomes of these interactions (global warming or cooling), fundamental properties of the molecules must be known. This experiment is being conducted with the intent of classifying the following fundamental properties of the molecule acetylene (H-C=C-H): identification of the regions of shape resonances and also collection of more finely resolved data corresponding to excited states below the ionization threshold of the carbon 1s core electron (291.1 eV). Soft x-rays from the Advanced Light Source are used to excite a carbon core electron, and our endstation, the magnetic mass spectrometer (MMS), is used to collect the subsequent products of the unstable excited acetylene. These products are ionic fragments that are collected via tuning the magnetic field on the MMS in order to select for a mass-to-charge ratio corresponding to an individual ionic fragment. Analysis of the excited states below the ionization threshold of the ionic fragments has reassigned two peaks previously identified as Rydberg states to actually be s* states. Analysis of above ionization threshold spectra has failed to identify regions of shape resonance simply because identification relies upon comparison of cation with anion spectra, and no anions were found.

A Fuel Efficient Plasma Thruster for Interplanetary Travel, *HANNA SMITH (Smith College, Northampton, MA 01063) F.R. Chang-Diaz (Johnson Space Center, Houston, TX 77059) D. A. Rasmussen (Oak Ridge National Laboratory, Oak Ridge, TN 37830).*
Fuel efficiency is a major pit fall in schemes for interplanetary travel, making even trips to nearby Mars unreasonable with current propulsion technologies. Conventional rockets must burn large quantities of chemical propellants in order to transport humans across interplanetary distances. This illustrates the basic trade-off between a rocket's thrust and its fuel efficiency. High-thrust systems, like chemical rockets, accelerate quickly but consume excessive fuel. Low-thrust systems take longer to speed up but are more efficient. A joint project between Johnson Space Center and ORNL is aimed at developing the Variable Specific Impulse Magnetoplasma Rocket (VASIMR) engine; a low thrust, fuel efficient propulsion system. In a VASIMR engine, radio waves ionize the propellant, hydrogen, to create a plasma discharge. Ions in the plasma are accelerated, then exhausted through a magnetic nozzle. While relatively little mass exits the nozzle, particles in the exhaust have high velocities. An experimental facility in the Fusion Energy Division includes several diagnostic instruments which collect data to optimize the plasma source for VASIMR. Optimization of an efficient plasma source is a prerequisite for developing a working VASIMR prototype.

The Potential Efficacy of an Energy Storage Cavity in the ALS. ROBERT HOCK (Stevens Institute of Technology, Hoboken, New Jersey 07030) ROBERT RIMMER (Lawrence Berkeley National Laboratory, Berkeley, California 94720).
The Touschek effect causes the electron beam at the Advanced Light Source to scatter in both the transverse and longitudinal directions. This is detrimental to the ALS users in that the beam lifetime is decreased and the transverse area of the beam is increased, resulting in a coarser light. A set of third harmonic cavities was installed to lengthen the electron bunches in the longitudinal direction and reduce this effect, thereby increasing the lifetime of the beam. Transients such as beam gaps cause cavity voltage to decay and grow in a saw-tooth waveform. In order to reach full benefit of the third harmonic cavities, the effect of the transients on the cavities must be reduced greatly. In order to do this, an energy storage cavity system has been proposed which would act as an electromagnetic flywheel that stores energy. The energy from this storage cavity would flood into the third harmonic cavity during beam gaps and reduce the magnitude of the variations. The result of coupling the energy storage cavity to the third harmonic cavity should likely reduce the effect of transients by a factor of at least four.

Radiation Effects Testing for Space Applications. *Teresa Bailey (Oregon State University, Corvallis, Oregon 97411) Dr. Peggy McMahan (Earnest Orlando Lawrence Berkeley National Laboratory, Berkeley, California 94720).*
Because of society's increased reliance on satellite technology for communication and entertainment purposes, space related industries have expanded beyond defense applications. Today, private corporations who are interested in making a profit make many of the spacecraft and satellites produced, in part or in whole. As a result, in order to keep prices down, these private companies do not use radiation hardened electronics, which were once the standard for all defense spacecraft. Instead, these companies opt for the regularly produced electronics, with unknown radiation hard characteristics, which increases the chances

for damage to the spacecraft in the harsh radiation environment of space. For this reason, the testing of these electronics to insure radiation hardness under certain radiation conditions, has become a widespread experiment in the space electronics industry. The 88-inch cyclotron at Lawrence Berkeley National Laboratory has the capability to simulate the proper radiation and environmental conditions for radiation effects testing, known as Single Event Effects testing. Because of its Electron Cyclotron Resonance sources, the 88-inch cyclotron is able to produce cocktails of ions, which are mixtures of many different ions spanning much of the periodic table. Also, the Aerospace Corporation has built an extensive testing facility in cave 4b of the cyclotron, which contains dosimetry, beam diagnostics, motion control, and vacuum chamber capabilities. A computer program that was also written by the Aerospace Corporation controls this testing facility. Aerospace has given LBL the permission to allow other companies to use their facility and has provided a version of their software. However, the software is unreliable and often quits working in the middle of an experiment. For this reason, I began writing a new computer program that would interface with the Aerospace test facility in cave 4b, but also be more user friendly to non-Aerospace users, and easily modified by LBL employees.

ALS Energy Storage Cavities. *Daniel Bowring (The College of William and Mary, Williamsburg, Virginia 23187) John Corlett (Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA 94720)*
Electrons travel around the Advanced Light Source storage ring in discrete groups, or bunches. To increase the lifetime of the bunches, and consequently to allow the users more beam time, the bunch density can be lowered by increasing the transverse cross section of the beam. However, this increases the cross-sectional area of the beam that falls on the target (spot size). Third-harmonic cavities were installed to expand the bunch longitudinally, which lowers the density while maintaining a small spot size. The cavities are passive so when the beam gap passes through, energy is lost. The exponential growth and decay of energy within the cavity means that different bunches experience different amplitudes and phases. To reduce this transient response, an energy storage cavity was designed to couple to the third-harmonic cavities. The energy storage cavities act as an energy reservoir, keeping the energy in the third-harmonic cavity closer to a constant value. A simple aluminum pillbox-type cavity was designed and fitted onto a spare third-harmonic cavity to test the properties of a coupled-cavity system. Simulations were run on MAFIA and the physical system was studied using a network analyzer. It was determined that adding the energy storage cavity decreased the system's R/Q by a factor of four or more. Also, the shunt impedance of the new system places no new power dissipation requirements on the existing cavities. It is very probable then, the addition of energy storage cavities will significantly lower the transient response of the present third-harmonic cavity system.

ALS Beamline 7.3.1.1 Software Optimization and Process Automation Software *Omar Cardona, Inter American University of Puerto Rico, Aguadilla, Puerto Rico, 00603 Andreas Scholl, E.O. Lawrence Berkeley National Laboratory, Berkeley, CA 94720*
The Advanced Light Source at the Ernest Orlando Lawrence Berkeley National Laboratory is a state of the art end synchrotron radiation source used for experiments in Materials Science Environmental Sciences and Biology. Of the various soft x-ray beam lines located at the electron storage ring, beamline 7.3.1.1 houses the second-generation PhotoEmission Electron Microscope (PEEM2) for real-time full-field imaging and spectromicroscopy of polymers and ferromagnetic materials. Operation of the PEEM2, equipment, settings processes, and image acquisition require user interaction with numerous computers, applications, and hardware. After analyzing the various processes used to operate the PEEM2, it was observed that direct communication between Image-Pro and LabVIEW applications was not possible due to the lack of support for TCP/IP within Image-Pro. Although Image-Pro does provide support for data extraction via DDE communications protocol, custom programs were needed to interconnect all applications and hardware to automate the multiple processes. Using AutoPRO, an Image-Pro SDK, it was possible to customize the application creating new programs and functions through the use of the IPBasic macro language. Using IPBasic to communicate with PEEM_Control.vi,, also a custom LabVIEW program, via DDE and then converting all to TCP/IP, it was possible to interconnect all hardware and software creating a faster and more efficient fully automated equipment setting and image acquisition process, with minimal user interaction while reducing the possibility of operator errors.

Data Reduction for the Supernova Cosmology Project. *Sterling Garmon (University of North Carolina at Chapel Hill, Chapel Hill, North Carolina 27514) Robert A. Knop Jr. (Lawrence Berkeley National Laboratory, Berkeley, California, 94720).*
The Supernova Cosmology Project has been using type Ia Supernovae as standardized astronomical phenomena in order to determine values for the cosmological constant and the mass-density constant. Before data from astronomical observations can be used for analysis, the data must be reduced. This must be done such that the quality of the image is maximized, while the noise in the image is minimized. The process of data reduction for ground-based deep-space observations is discussed.

STAR Preliminary Results in Au + Au Collisions at s = 130 A GeV. *Matthew Goupell (Hope College, Holland, Michigan 49423). Nu Xu (Lawrence Berkeley National Laboratory, Berkeley, California 94702).*
The recent construction of and first collisions at the Relativistic Heavy Ion Collider (RHIC) move the threshold of high-energy nuclear physics to a new and exciting level. The main goal of RHIC is to search for the formation of quark-gluon plasma, a theoretical phase of matter that consists of individual partons. By using the STAR, the charged particles in the collisions were measured to gain a fundamental understanding of the detector performance and physics of relativistic nuclear collisions at s = 130 A GeV. This study measured the charged particle ratios for π^-/π^+, K^-/K^+, and pbar/p. Although this is a preliminary study and several corrections are needed, the results show that the net baryon density is not zero and several model predictions can be eliminated.

The Blue Blob Galaxies: Evidence for Ram Pressure Stripping. *Rachel Mason (Brown University, Providence RI, 02912) and Greg Aldering (Lawrence Berkeley National Laboratory, Berkeley CA, 94720).*
The Blue Blob galaxies are blue spiral galaxies that are located near the center of a dense group of red elliptical galaxies known as the Coma cluster. Because of their unusual surroundings, it is possible that the Blue Blob galaxies may provide an example of a hypothesized phenomenon known as ram pressure stripping. Ram pressure stripping occurs when the gas in a galaxy cluster initially causes galaxies entering that cluster to increase star formation. When the pressure of the gas in the cluster becomes greater than the restoring pressure of the galaxy, the gases are stripped out of the galaxy and star formation ceases. Subsequently, the massive blue stars in the galaxy die, leaving only red stars like those seen in most Coma cluster galaxies. Spectrophotometric data for 23 of the Blue Blob galaxies was reduced, and redshifts were calculated for 22 of these galaxies. Further research will provide exact redshifts for these 23 galaxies and information about their star-formation rates. That information will be a good indicator of whether or not the Blue Blob galaxies are experiencing ram pressure stripping.

RK-TBA. *Susan Hunter (North Carolina State University, Raleigh, North Carolina, 27607) Tim Houck (Lawrence Livermore National Laboratory, Livermore, California, 94550) and Steven Lidia (Lawrence Berkeley National Laboratory, Berkeley, California, 94720).*
The RK-TBA group at Lawrence Berkeley National Laboratory seeks to create a more efficient linear particle accelerator using rf and induction technology. Linear accelerators, or "linacs", are used in the study of high energy physics, where researchers attempt to determine the fundamental building blocks of matter and research the four basic forces: gravitational, weak, electromagnetic, and strong. In order to research particle interactions at higher and higher energies, efficient accelerators that can produce particle center of mass collisions at 1TeV and beyond are thought to be necessary. To power their high peak power induction linac, the RK-TBA group uses a pulsed power system that applies a voltage to a circuit that, in turn, powers the beam. Pulsed power systems are made up mainly of LRC circuits, which are circuits containing inductors, resistors, and capacitors. During my work with the RTA group, I helped build and test inductance cores made of METGLAS, a magnetic alloy, and Mylar, an insulator, wound around PVC pipe. These cores were tested to find the value of their volt-seconds and were sorted such that, when placed on the accelerator in pairs, the effectiveness of their inductances was optimized.

Photoionization with an Advance Light Source *KRISTEN LANTZ (Grinnell College, Grinnell, IA 90112). FRED SCHLACHTER (Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA 94720)*
Air-born pollutants released by cars and industries tend to rise into the upper atmosphere where they can interact with photons from the sun.

This reaction then produces additional molecules that can react with ozone or other compounds in the air and contributes to "global climate change." To more clearly understand how these processes occur and what factors affect them, the fundamental processes of molecules are researched. We studied the photoionization of acetylene and the fragments produced to learn more about reaction pathways this molecule could initiate or be involved in. Beamline 8.0.1 at the Advance Light Source was used with a Magnetic Mass Spectrometer endstation. Data were collected for nine ion fragments through a broad range of photon energies, from 284-320 eV, encompassing the carbon k-shell ionization threshold for acetylene. The partial ion yields we produced reflect the core-level spectroscopy of acetylene and reveal the location of the p* states, the Rydberg states, the s* states (previously incorrectly assigned), doubly excited states, and the shape resonance region. In the future, coincidence experiments promise to shed more light on the decay processes that produce these ions.

Photoionization of inert gases using synchrotron radiation and electron spectroscopy *Benny Ng[1], György Snell[2, 3], John Bozek[3] [1] University of California-Los Angeles, Department of Chemistry and Biochemistry, Los Angeles, CA 90095 [2] Western Michigan University, Department of Physics, Kalamazoo, MI 49008 [3] Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720*
This paper is divided into introduction, experimental procedures, theory, my role, result and conclusion. The introduction contains a history of the photoelectric effect, photoionization, and Auger decay and our experiment setup and our purpose of studies. The work studies photoionization and Auger decay in inert gases as a function of the photon energy. We examined the angular distribution of photoelectrons with a given photon energy. Experimental procedures begin with synchrotron radiation at Advanced Light Source, two beamlines that I worked with, and two types of electron spectrometers. Theory focuses more in depth on photoionization, different Auger decay transitions, and spin polarization using Mott polarimeter. Then, I describe my involvement in the research in three main areas: vacuum setup, electrical setup, and data acquisition. Lastly, results and conclusions explains photoabsorption and resonant Auger decay spectra. The significance of our research is to compare our experiment with the same experiment in the journal and to formulate a better measurement with better data.

Superconducting Magnet Development Using ANSYS. *JO ANN DACANAY and Dr. Daniel Dietderich (Superconducting Magnets Group Lawrence Berkeley National Laboratory, Berkeley, CA).*
In the high field magnet program at Lawrence Berkeley National Laboratory, accelerator magnet prototypes are designed with epoxy impregnated niobium-tin and niobium-titanium superconductor. Accurate mechanical property values are essential for magnet mechanical design and prediction of conductor performance. The measurements are made in compression and are conducted in three orthogonal directions. The key property value measured on coil samples is the modulus of elasticity. Another important application for design is the contact elements. By applying these to our composite Nb3Sn sample, we will be able to determine the critical current at a given stress and strain. This will be done using the ANSYS program.

Upgrade and Analysis on RTA's Diagnostic System. *Shawn Putnam University of Minnesota Duluth (UMD) Duluth MN. Tim Houck Lawrence Livermore National Laboratory Livermore CA. Steven Lidia Lawrence Berkeley National Laboratory Berkeley CA.*
An induction accelerator has the capability to accelerate "high current" particle beams to relativistic energies within short linear distances. This ability not only makes them favorable power sources in the future high-energy particle-antiparticle colliders, but also makes them an attractive tool in the studies on high-energy high-current beam dynamics. However, before scientists can efficiently apply induction accelerator technology to energy source purposes, many challenging problems need to be answered. Such studies are extremely difficult due to the high dimensionality of the problems. Presently, the RTA facility at LBNL has commissioned the electron beam injector and is studying the challenging beam dynamics. In these studies a major concern is the accuracy with which experimental measurements can be made. For this reason, the work conducted during this summer's internship comprised of three main parts related to the analysis and calibration of RTA's beamline diagnostic system.

Characterization of a High Thermal Conductivity Carbon Foam. *Brian Dill (Carson-Newman College, Jefferson City, TN 37760) David Stinton & James Klett (Oak Ridge National Laboratory, Oak Ridge, TN 37830).*
Heat management is an issue of utmost importance in both the electronics and automotive industries. A mesophase pitch-based graphitic foam has been developed at Oak Ridge National Laboratory that promises to increase the effectiveness of heat exchangers and heat sinks, while decreasing their size and weight. Determining the effects of differing preparation techniques on the material's structure is vital to increasing the material's durability and further improving the materials thermal conductivity. The relationships between three groups of variables were explored: changes in graphitizing temperature/time/pressure, cell/crystallite structure, and the final product's tensile strength and thermal conductivity. Cell and crystallite structure were determined by use of a scanning electron microscope, an optical microscope, and x-ray diffraction. Tensile strength was measured using an Instron device, while the samples' thermal conductivities were found by the xenon flash diffusivity technique. Research concluded the effects on specific production specifications towards larger, more interconnected pores and ligaments of better organization, as well as the increase of tensile strength by polymer densification.

Superconducting Magnets Research. *LUIS A. SOTO ROSADO (University of Puerto Rico, Mayaguez Campus, Mayaguez, Puerto Rico 00680) RAY HAFALIA/STEVE GOURLAY (Lawrence Berkeley National Laboratory, Berkeley, California 94704).*
The Superconducting Magnets Group of the AFRD (Accelerator and Fusion Research Division) takes a vertically integrated approach by offering expertise "from melt to magnet"—that is, at all phases from basic development of better superconducting materials to evaluation of finished magnets. Researchers at the Lawrence Berkeley Lab have shattered the world record for field strength in a dipole magnet. At this time the Superconducting Magnet Group is developing a new design of dipole magnet. This design is base on planar coils in the shape of a racetrack, called RD3 (RaceTrack Dipole—third generation). Pro/ENGINEER® 3D Modeling System is providing this Project the latest technology and capabilities for high quality components and the finest detailed design. This is a nice example of what science and computers are doing.

Characteristics of a Rotating Arc Spark Plug. *DARREN O'CONNOR (North Carolina State University) John Whealton, Ph.D. (Engineering Technology Division , Oak Ridge National Laboratory, Oak Ridge, TN 37830)*
The properties of arc plasmas rotating due to applied magnetic fields were investigated. The development of spark plugs that are more efficient and reduce emissions at the same time is the overall goal. Techniques used to date include a high speed framing camera, a digital video camera, oscilloscopic current traces as a function of time, and spectroscopic analysis of Ar and Cu in the plasma. The device used to produce the phenomenon is a rotating arc spark plug (RASP). It is proposed that such a device would 1) increase the volume occupied by the spark and 2) lead to higher plasma temperatures, which should result in improved efficiency and reduced emissions. Preliminary results seem to indicate that both characteristics are present in the RASP.

WASTE MANAGEMENT

Individual Reactions of Permanganate & Various Reductants. *AMBER M. GAUGER (Lewis-Clark State College) Richard Hallen (Chemical Process Development Group at Pacific Northwest National Laboratory, Richland, WA 99352)*
Tank waste on the Hanford Site contains radioactive elements that need to be removed from solution prior to disposal. One effective way to do this is to precipitate the radioactive elements with manganese solids, produced by permanganate oxidation. When added to tank waste, the permanganate, Mn(VII), reacts quickly producing manganese (IV) dioxide precipitate. Because of the speed of the reaction it is difficult to tell what exactly is happening. Individual reactions using non-radioactive reductants found in the tanks were done to determine reaction kinetics, what permanganate was reduced to, and what oxidation products were formed. In this project sodium formate, sodium nitrite, glycolic acid, glycine, and sodium oxalate were studied using various concentrations of reductant in alkaline sodium hydroxide solutions. It was determined

that formate reacted the quickest, followed by glycine and glycolic acid. Oxalate and nitrite did not appear to react with the permanganate solutions. The formate reactions quickly reduced permanganate, Mn(VII), to manganate, Mn(VI), and then to manganese (IV) dioxide. These reactions oxidized formate to carbonate and water. The glycolic acid was oxidized slower producing oxalate, water, and manganate, which would disproportionate to permanganate and manganese (IV) dioxide solids. The rate at which Mn(VI) disproportionates is usually slower than the rate at which Mn(VII) is reduced to Mn(VI), however in this case the rates were about equal. The glycine reactions formed some ammonia in solution, oxalate, and water. They reacted similar to the glycolic acid reactions, producing manganese dioxide precipitate before the solution turned totally green from Mn(VI). The formate reactions consumed one mole of hydroxide for every 3 moles of formate, while the glycolic acid and glycine reactions consumed 7 moles of hydroxide for every 3 moles of reductant. These reactions should help to determine the majority of products found in a mixture of these solutions.

Investigation of Contaminant Species at the Bacteria-Geosurface Interface, *KEVIN GERMINO (College of the Holy Cross, Worcester, MA 01610) Ken Kemner (Argonne National Laboratory, Argonne, IL 60439)*
Understanding the interactions of metal contaminants in the environment is of fundamental importance in the development of remediation techniques. The use of bacteria and their extracellular material are thought to play a key role in determination of a contaminant's fate in the microenvironment. Using hard x-ray microimaging, we can investigate these interactions by observing the spatial distribution of both naturally occurring metals and contaminant metals at the microbe's interface with its local microenvironment. This paper presents an introduction to bioremediation, an outline of the methods utilized at Argonne National Laboratory, and some of our findings with respect to chromium's behavior at the microbe-contaminant interface.

Seismic Monitoring and Analysis Using the Earthworm System. *DENNIS GRAHAM (Washington State University, Pullman, WA 99164) B. Moon (Pacific Northwest National Laboratory, Richland, Washington 99355).*
Seismic activity has the potential to damage radioactive material storage tanks and facilities at the Hanford Site. In order to protect the Site against seismic hazards, continuous earthquake and activity data must be available to analyze and anticipate seismic hazards. Furthermore, during disasters, information on earthquake strength and duration must be available to estimate damage inflicted upon buildings and waste storage facilities.

SCIENCE POLICY

Students Must Think to Learn: Instructional Reform in Science Education. *Kathleen Donoghue (Columbia University, New York, NY 10027) Fernando Cajas (Project 2061 of the American Association for the Advancement of Science, Washington DC 20005).*
Instructional reform of math, science and technology education is necessary for students to learn more effectively in the light of new content reform. Content reform has placed emphasis on knowledge as an understanding of concepts and ideas, not merely a set of facts. Due to this new content focus, instructional methods are being reformed from the teacher-tell and student-memorize method to a method that allows students to think. It is necessary to think in order to learn. Teachers must learn to use methods that promote student thinking by allowing students to solve challenging problems and ask questions. Instructional reform is a slow process because teaching is a cultural activity that is difficult to change. However, the instructional methods of Japanese teachers can be used as a guide for instructional reform.

Establishing the Office of Research on Women's Health. *Katie Sokolski (Wellesley College, Wellesley, MA 20481) S.R., C.M, S.W. P.F. (DOE Headquarters, Washington D.C. 20585).*
The Office of Research on Women's Health (ORWH) was legally established in 1990 within the Office of the Director of National Institutes of Health (NIH) as a result of the preliminary hearings leading to the *NIH Revitalization Act of 1993*. Its primary function is to advise the Director and staff of NIH on matters relating to research on women's health. Their goal is to strengthen and enhance research related to diseases, disorders, and conditions that affect women, as well as co-fund research on women's health issues. The office has established and works to maintain a policy that ensures that women are appropriately represented in research conducted and supported by NIH. They create opportunities for and support recruitment, retention, reentry, and advancement of women in biomedical careers (Pinn, 2000). Official United States documentation as well as ORWH documentation was used to research the history and legal establishment of ORWH.

Block Training. *KATIE JO JOHNSON (Brigham Young University) No Mentor Listed (Idaho National Engineering and Environmental Laboratory, Idaho Falls, Idaho 83415)*
This summer I worked for INEEL Training Department. One of my main projects was to put together and implement site wide Block Training. In its simplest form, block training is the grouping together of similar courses into one main training session. Currently, employees are pulled from their jobs several times a year to attend training. Not only does this interrupt an employee's workday, it also costs the INEEL a great deal of money in travel time. Therefore, the purpose of block training is to create blocks of training containing all of the courses an employee would need for the entire year, in an effort to save money and increase worker productivity. In order to implement these training blocks, I first had to research out what courses were taken most frequently. I found these courses by comparing and contrasting training matrixes from each INEEL facility. I then looked through training reports to determine which employees needed to take these courses. Lastly, I put the courses and the corresponding employees into a database so I could run specific queries. I had to take into account the frequency and length of each course and determine a logical way of grouping these courses together. After many attempts and much analyzing, I was able to produce a three-day training session containing 10 classroom and 7 computer-based courses that would apply to the general INEEL population. Not only will this training session save time and money, it will also increase instructor availability and decrease scheduling difficulties

The National Energy Security act of 2000 – The Issues and Players. *Derek Swick (Juniata College, Huntington, PA, 16652). Becky Fliss (University of Texas, Austin, 16652), DOE Headquarters, Washington D.C.*
The political influence of the oil and gas industry on congressional legislation is examined, specifically the National Energy Security act of 2000 (S.2557). Using oil and gas Political Action Committee and individual contributions based on recent Federal Election Commission data, the co-sponsors of S.2557 are found to receive more money from the oil and gas industry than a control group of eight random senators. Co-sponsors of the bill are found to receive an average of $127,801 while the control group is found to receive $46,149. Statistical significance using the Mann-Whitney U Statistical test is found between the campaign contributions received by both groups, with 96 per cent confidence that the control group received significantly less money in contributions than the co-sponsors.

Energy End-Use Forecasting. *MICHELE THOELE (the University of Illinois, Urbana/Champaign, IL 61820) JONATHAN KOOMEY (Lawrence Berkeley National Laboratory, Berkeley, CA 94702)*
Energy End-Use Forecasting plays an essential role in policy making. The Environmental Protection Agency, as well as the Department of Energy, supports many programs, such as the Energy Star program and research endeavors to make good energy use policy decisions. In the Environmental Energy Technologies division of the Lawrence Berkeley National Laboratory, there are many scientists whose work is dedicated to the Energy Star program. One aspect of this work is a web site called the Home Improvement Tool that will be launched by the E.P.A. in early October. This web site and others that my group runs are where I did most of my work this summer.

GENERAL SCIENCES

Demand for Energy as Related to Ambient Air Temperatures in California's Free Power Market. *ELIZABETH ALFORD (University of Idaho) Robert J. Turk (Idaho National Engineering and Environmental Laboratory)*
California is the leader in the production of geothermal power, which is becoming an increasingly viable alternative energy source. One important goal of the DOE is to see that the potential of geothermal energy is realized on the world market. In light of California's recent move to a

deregulated power market, predicting the demand for power becomes essential for Californian geothermal plants to maximize output at peak times and thus maximize profits. It is thought that there is a direct correlation between demand for power and weather conditions. Hourly ambient air temperatures for San Francisco, Sacramento, and Los Angeles, as well as load factors for California were gathered via the Internet. They were then plotted month by month for each city, and it was found that temperature and load are indeed very closely correlated. Both temperature and load appear to follow a daily schedule; they both peak in the late afternoon and fall to their low in the early morning between three and six a.m. The load also peaks a second time in the late evening around nine or ten p.m. when people turn on their lights and televisions. This is more noticeable during the winter because it is dark for more hours in a day. During the summer months, load is more susceptible to change as the temperature changes due to the use of air conditioners. While there is a definite correlation between ambient air temperature and load, the extent of the causal effects are uncertain. There is a lack of complete temperature data, and the load information is only given for the whole state, not broken into zones. As time goes on and more data is collected, a better picture of the relationship between demand and ambient air temperature can be determined.

Advancing Stewardship: A GIS Application for Documentation and Location Of Cultural Resources. *Sera White(Idaho State University, Pocatello ID, 83201) Randy Lee (Idaho National Engineering and Environmental Laboratory, Idaho Falls ID, 83402)*
The main objective of this project was to develop a fully integrated automatic system for accessing and archiving information on the INEEL Cultural Resources, using Microsoft Access and ESRI ArcView. This would make archive searches more efficient and thorough, as well as enhancing customer service and overall management of the resources. The first task was to analyze the CRM system and processes for storing information. The next step was to create fields and tables. After the fields and tables were created, automated data entry forms were created. The last step in completing the database design was to make reports. Future work includes writing the ESRI Arcview application.

GIS Internship at PNNL's Marine Research Laboratory. *ARTEMIO SANCHEZ (Heritage College) Karen Steinmaus (Environmental Technology Division, Marine Research Laboratory, Pacific Northwest National Laboratory, Sequim, WA 98382)*
During my internship at the Pacific Northwest National Laboratory (PNNL) from June 13 to August 4, I had the opportunity to work in the GIS lab conducting various tasks assigned by my mentor Karen Steinmaus. I had the option of selecting tasks that best matched my experience and interest. I started by learning ArcExplorer, a geographic information application and its functions and the purpose for which ArcExplorer intended to be use. Other projects included conducting web searches and participating in research projects on water quality. These gave me a broader perspective of the science conducted at PNNL's Marine Research Laboratory.

Delta Q Test for Determining Duct Leakage. *Wempen, J. Lawrence Berkeley Lab, Berkeley, CA.*
The Delta Q test is a recently developed diagnostic test for determining duct leakage in finished houses. Duct leakage represents the combined effects of pressure, leak size, and leak geometry. Wind affects the repeatability of duct leakage testing, because it causes random, non-uniform, and rapidly changing pressures over the building envelope that are used in the DeltaQ test procedure. Based on 20 repeated tests of a mobile home trailer at Lawrence Berkeley National Laboratory under various wind conditions, the DeltaQ test has reasonable repeatability.